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NATO Committee on the Challenges of Modern Society

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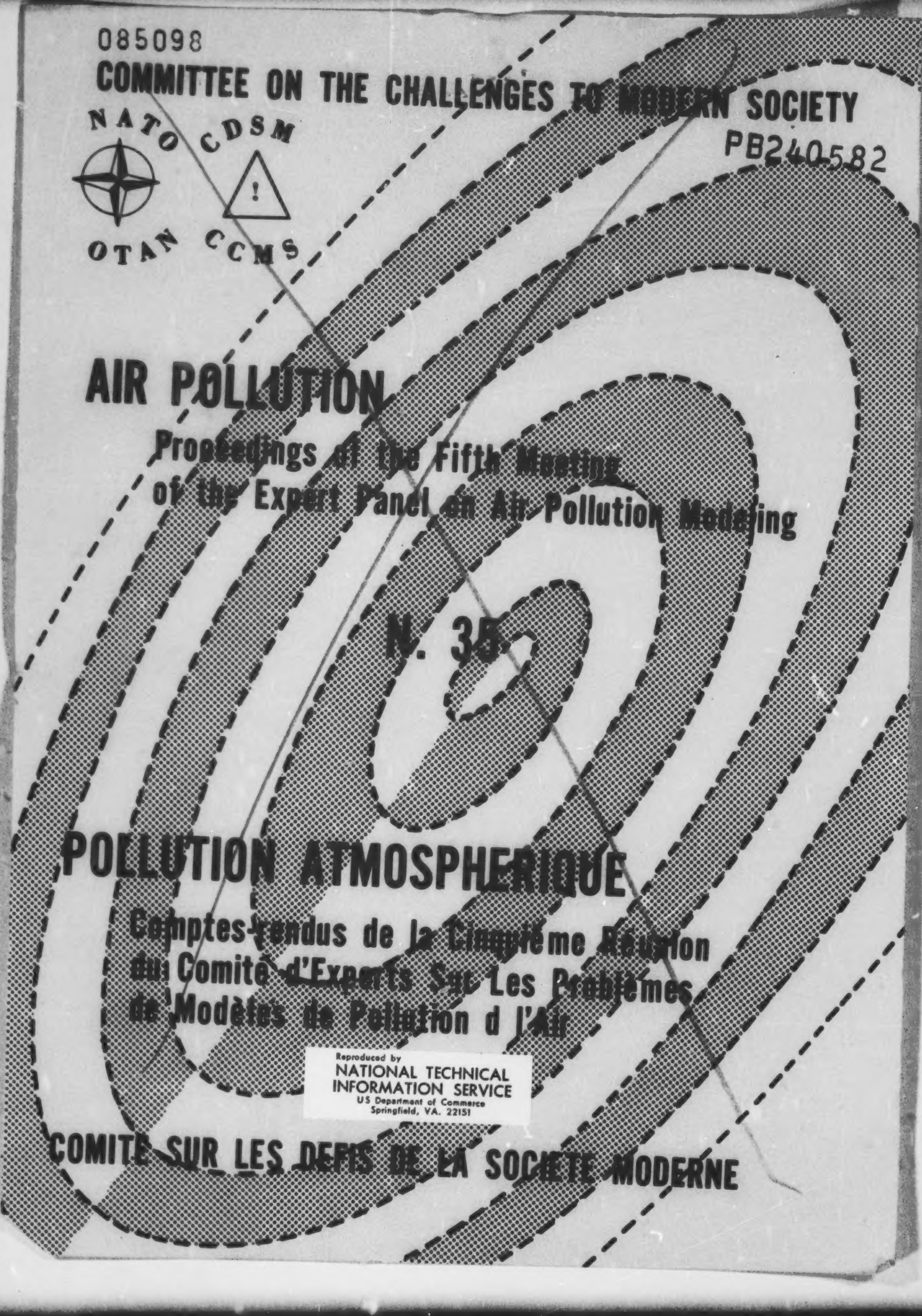

AIR POLLUTION

Proceedings of the Fifth Meeting of the Expert Panel on Air Pollution Modeling

N. 35

POLLUTION ATMOSPHERIQUE

Comptes-rendus de la Cinquième Réunion du Comité d'Experts Sur Les Problèmes de Modèles de Pollution d l'Air

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A REPORT OF THE AIR POLLUTION PILOT STUDY,
NATO COMMITTEE ON THE CHALLENGES OF MODERN SOCIETY

August 1974

OTHER NATO/CCMS AIR POLLUTION PUBLICATIONS

Technical Report on the Conference on Low Pollution Power Systems Development, N.4

Proceedings of the Second Meeting of the Expert Panel on Air Pollution Modeling, N.5

Guidelines to Assessment of Air Quality (Revised) SO_x, TSP, CO, HC, NO_x and Oxidants, N.6*

Air Quality Criteria for Sulfur Oxides, N.7*

Air Quality Criteria for Particulate Matter, N.8*

Air Quality Criteria for Carbon Monoxide, N.10*

Control Techniques for Sulfur Oxide Air Pollutants, N.12*

Control Techniques for Particulate Air Pollutants, N.13*

Proceedings of the Third Meeting of the Expert Panel on Air Pollution Modeling, N.14

Air Quality Criteria for Nitrogen Oxides, N.15*

Control Techniques for Carbon Monoxide Emissions from Stationary Sources, N.18*

Control Techniques for Hydrocarbons and Organic Solvent Emissions from Stationary Sources, N.19*

Control Techniques for Nitrogen Oxide Emissions from Stationary Sources, N.20*

Air Quality Criteria for Photochemical Oxidants and Related Hydrocarbons, N.29**

Proceedings of the Fourth Meeting of the Expert Panel on Air Pollution Modeling, N.30

Symposium on Low Pollution Power Systems Development, N.32

*Also available in French
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PROCEEDINGS OF THE FIFTH MEETING OF THE EXPERT PANEL ON AIR POLLUTION MODELING

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PREFACE

At the 4th Meeting of the NATO/CCMS Expert Panel on Air Pollution Modeling (Oberursel, W. Germany, 28-30 May, 1973) a workshop on the applications of modeling and users' needs occupied the whole of the first day. This very strongly emphasized the need for improving the communications between the designers of air quality models, and the users or decision makers in the air quality management process. In a preliminary attempt to remedy this situation a one and one-half day "modeler-user" workshop was included for the 5th Meeting of the Panel, that was held 4-6 June, 1974 at the Danish Atomic Energy Commission Research Establishment Risø, Roskilde, Denmark. A U.S. invitation was also made at the CCMS Plenary on 7-8 May, 1974 in Turin, Italy, to send policy level air pollution officials to this workshop, although this appeared to have produced only a weak response. The remaining period of the 5th Meeting was devoted to the presentation of papers and discussion of five technical items relating to air quality modeling. These were: the development of a common data base for air quality modeling, the validation of air quality simulation models, short-term and real-time modeling, the modeling of complex topographic effects, and recent developments in air quality modeling.

Like several of the earlier meetings of the NATO/CCMS Panel on Modeling, the 5th Meeting was one of wide participation in order to encourage a maximum exchange of information on a broad international basis. Sixty-seven individuals attended the meeting, representing fourteen countries as follows: U.K. (4), Spain (1), Norway (2), Sweden (3), Denmark (20), Italy (4), France (2), The Netherlands (5), Belgium (3), Switzerland (2), W. Germany (8), Canada (2), Turkey (1), U.S.A. (10). Invitations to participate had also been sent to representatives in the U.S.S.R., Hungary and Japan. Exceptionally fine facilities were made available for the three-day meeting. Special thanks are due to the Danish Atomic Energy Commission Research Establishment Risø and to Dr. Niels E. Busch and his staff of the Physics Department, for acting as hosts for the meeting and making all the many arrangements required in its support.

The present document contains the reports of the several rapporteurs to the different sessions of the meeting, together with the papers that were presented or made available in support of the discussions. Due to the quite enthusiastic response of the participants and the quite limited time that was available, it was unfortunately not possible in every case to provide time for an oral presentation. Also in order to accommodate some papers that only became available after the start of the meeting, it was necessary, in some cases, to fit these in without proper regard to the primary topic under discussion.

K. L. Calder

Kenneth L. Calder, Chairman
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Chapter 1

AGENDA

5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

AGENDA

5th MEETING OF NATO/CCMS EXPERT PANEL ON AIR POLLUTION MODELING

June 4-6, 1974

Danish Atomic Energy Commission Research Establishment Risø

Roskilde, Denmark

Tuesday, June 4 - 0900-1230

Welcoming Remarks - K. L. Calder & N. Busch: 0900-0915

Item 1 - Modeler-User Workshop: 0915-1230

Chairman - Dr. N. Busch (Denmark)

(a) Introductory Remarks - K. H. Jones (U.S.A.)

(b) The Air Quality Management Concept - K. H. Jones (U.S.A.)

(c) Some Canadian Activities - M. Kwizak (Canada)

(d) Miscellaneous Questions Relating to the Use of Air Quality Simulation Models - K. L. Calder (U.S.A.)

(e) Applications of Models to the Solution of the Problem of A.Q. Maintenance - H. Fortak (F.R.G.)

COFFEE: 1050-1100

(f) Special Applications of A.Q. Models by EPA and Modeling Analysis for Implementation Planning Program - H. H. Slater (U.S.A.)

(g) Use of Dispersion Models During Planning Phases of Industrial & Domestic Regions - L. Kropp (F.R.G.)

(h) Requirements of A.Q. Models for Land Use Planning - K. E. Gronskei (Norway)

Tuesday, June 4 - 1400-1730 hrs.

Item 1 - Modeler-User Workshop (cont.)

Chairman - Dr. K. H. Jones (U.S.A.) (Rapporteur: L. E. Niemeyer)

(a) Rollback - H. H. Slater (U.S.A.)

(b) Point-Source Plume Models - H. H. Slater (U.S.A.)

COFFEE: 1530-1540

(c) Multiple Source Urban Models - H. H. Slater (U.S.A.)

(d) The Users Need for Precise Description and Verification of a Model - A. Corlin (Denmark)

(e) Open Discussion

Wednesday, June 5 - 0900-1230 hrs.

Item 1 - Modeler-User Workshop (cont.)

Chairman - Dr. E. Weber (F.R.G.) (Rapporteur: D. G. Fox)

(a) Line Source Models - L. E. Niemeyer (U.S.A.) (paper by D. B. Turner)

(b) A Rational Air Pollution Surveillance Network Design - R. Lafleur (Canada)

(c) Application of the Tikvart-Martin Model to the Frankfurt Area in Comparison with Results of the Hanna-Gifford Model - J. Strott (F.R.G.)

COFFEE: 1050-1100

(d) Episode Planning - L. E. Niemeyer (U.S.A.)

(e) A Preliminary Investigation of the Air Pollution Problem in Venice - E. Runca (Italy)

(f) Open Discussion

Wednesday, June 5 - 1400-1730 hrs.

Item 2 - Development of a Common Data Base for Air Quality Modeling: 1400-1530

Chairman - Dr. W. Klug (F.R.G.) (Rapporteur: S. E. Larsen)

(a) Considerations Based on the U.S. Regional Air Pollution Study (paper by R. E. Ruff) - D. G. Fox (U.S.A.)

(b) Verification of the Gaussian Plume Model - L. E. Olsson (Sweden)

COFFEE: 1520-1530

Item 3 - Validation of Air Quality Simulation Models: 1530-1730

Chairman - Dr. L. E. Olsson (SWEDEN) (Rapporteur: P. Roth)

(a) Validation and Sensitivity Analysis for Gaussian Plume Urban Diffusion Model (Geomet, Inc., Rockville, Md.) - K. L. Calder (U.S.A.)

(b) Computing Optimal Air Pollution Abatement Strategies - S. A. Gustafson (Sweden)

(c) Open Discussion

Thursday, June 6 - 0900-1230 hrs.

Item 4 - Short-Term and Real-Time Modeling: 0900-1100

Chairman - L. E. Niemeyer (U.S.A.) (Rapporteur: K. Grønskei)

(a) Applications of Modeling for Supplementary Control Systems - B. Egan (U.S.A.)

(b) On the Lognormal Distribution of Air Pollution Data - D. T. Mage (Denmark)

(c) The Relations Between Air Pollution Concentrations, Averaging Times and Frequency Distributions - S. E. Larsen (Denmark)

(d) Open Discussion

COFFEE: 1050-1100

Item 5 - Modeling of Complex Topographic Effects: 1100-1230

Chairman - Dr. A.W.C. Keddie (U.K.) (Rapporteur: F. B. Smith)

(a) Modeling Activities for Complex Terrain - D. G. Fox (U.S.A.)

(b) Description of a Study for a Site for a Future Power Plant - J. P. Granier (France)

(c) Open Discussion

Thursday, June 6 - 1400-1730

Item 6 - Recent Developments in Air Quality Modeling:

Chairman - Dr. C. A. Velds (The Netherlands) (Rapporteur: B. Egan)

(a) Research Program of Model Development Branch of EPA - D. G. Fox (U.S.A.)

(b) Assessment of Validity of Airshed Models - P. Roth (U.S.A.)

(c) Applications of Repro-Modeling in Air Modeling - W. S. Meisel (U.S.A.)

COFFEE: 1530-1540

(d) Dispersion from Tall Stacks - W. Klug (F.R.G.)

(e) Some Views on Modeling Dispersion and Vertical Flux - F. B. Smith (U.K.)

(f) Open Discussion

Chapter 2

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

PARTICIPANTS AT 5TH MEETING OF NATO/CCMS EXPERT PANEL ON AIR POLLUTION MODELING

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Roskilde, Denmark, 4-6 June 1974

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Chapter 3

OPENING (AND CLOSING) REMARKS

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

OPENING REMARKS

As Chairman it gives me the greatest pleasure to welcome such an impressive group of participants to the 5th Meeting of the NATO/CCMS Expert Panel on Air Pollution Modeling. [illegible] our first meeting, held in Frankfurt in 1970 under the Chairmans[illegible] Mr. R. A. McCormick, I believe there were only about fourteen o[illegible] present. As a rough guess I would say there are probably at least five times as many here today, and I see a large number of new faces as well as many old and familiar ones. This augurs well for the future of air pollution modeling and also for an unusually wide and intimate exchange of information on the subject. Let me also say right away that we have never before had such distinguished scientific surroundings as for our present meeting now being held in the Niels Bohr Auditorium at Risø. For this the thanks of all must go to Dr. Niels Busch for his efforts on our behalf and to the Danish Atomic Energy Commission Research Establishment Risø, for acting as hosts and providing such unusually fine facilities and arrangements for the meeting.

At the 4th Meeting of the Panel held in Oberursel, W. Germany in 1973, a one-day workshop session strongly emphasized the need to improve communications between the modeling scientist and the policy-making user. Dr. Kay Jones, the Director of the NATO/CCMS Air Pollution Project, will say more on this very soon. Suffice it to say here that a special attempt has been made to invite some major users for the present meeting, as a step towards establishing an interface and a basis for improved communications. This will be the primary goal for the modeler-user workshop that will occupy the first one and one-half days of the meeting, up to lunch-time tomorrow. It is hoped that this workshop will stimulate discussion between the "users" and "modelers" and illustrate to planners the unique potential of modeling for resolving a wide variety of problems in air quality management. The remaining one and one-half days of the meeting will be devoted to the discussion of five special technical topics, all related to air quality simulation modeling, and which seem to have wide interest at the present time. These five topics are the development of a common data basis for air quality modeling, the validation of air quality simulation models, short-term and real-time modeling, the modeling of complex topographic effects and recent developments in air quality modeling.

We have a very busy three days ahead of us and it was for this reason that a detailed and time-oriented agenda was prepared to guide the speakers and participants. This was not done without quite a little apprehension, as right up to the present time, I have had only rather general indications of potential speakers and of the titles of possible papers. Thus, in some cases, I may have to apologize for incorrect titles, or even worse, for not expressly including time for papers that may have been specifically prepared for the meeting, but of which I had no previous knowledge. In the latter case, I would particularly appreciate being informed by authors -- at the coffee break this morning -- and we will make every attempt to work all these papers into the discussions at the most appropriate times.

In addition to the papers there will, of course, be major value in the discussions that these stimulate. In order that there could be a fairly complete record of the discussions in our Proceedings, I last year proposed that discussants should leave notes of their actual contributions with me before the close of the meeting. This year, with a much enlarged gathering and a very tight schedule, I have asked for the help of some rapporteurs at the various sessions -- this, of course, in addition to the several session chairmen. I am also hoping that master copies, i.e., of a type suitable for reproduction, of any papers that have been prepared can be made available to me before the end of the meeting, or mailed to me not later than 30 June 74 for publication in the Proceedings.

I would now like to call upon Dr. Niels Busch, who I am quite certain will have many announcements for us. After these, and before starting the Modeler-User Workshop, we will ask participants now in the auditorium to introduce themselves individually by name and affiliation.

CONCLUDING REMARKS (6 June 1974)

In bringing this meeting to a close I would like to thank you all most sincerely for your many efforts to make it a success. These include such things as finding time to attend and participate, preparing special papers and presentations, entering wholeheartedly into the spirit of the discussions and helping as chairmen and rapporteurs. Once again I would also like to thank Dr. Niels Busch and his staff for their many efforts on our behalf at this meeting, and the Danish Atomic Energy Commission Research Establishment Risø for acting as hosts and making available such unusually convenient and impressive facilities.

I believe that the meeting has been one of the most successful to date and it is certainly a first in the positive attempt made to bridge the communications gap between the technical air quality modeling community and the policy-making planners. I also believe that all these meetings of the NATO/CCMS Panel on Modeling have demonstrated, beyond all shadow of doubt, the strongly beneficial effects of an informal and wide exchange of technical information on air quality simulation models, and I know that many valuable professional contacts have been established as a direct result of the meetings. We have heard from Dr. K. H. Jones that at the May 1974 CCMS Plenary, the delegates from the NATO member countries agreed that the activities of the Panel on Modeling should be continued. The Federal Republic of Germany, as one of the original copilot countries, has also agreed to introduce a follow-up initiative on air quality modeling and assessment at the next CCMS Plenary, for continuation of the joint efforts for at least another two years. The new effort will have as its primary task the provision of greater understanding and confidence to the policy makers who depend on the model results in the air quality management decision-making process. The two-year period will be used primarily to improve communications and provide closer contacts between the modelers and the users, through exchange of ideas, more complete discussion of users' needs, and demonstration of various modeling techniques. I am certain that I can speak for all of us here, in wishing the reorganized Panel every success. Personally, I have very much enjoyed the honor of being associated with the Panel on Modeling, and it has provided the basis for many close friendships that will continue into the future. May I wish you all bon voyage and good luck until we meet again. My good friend Niels Busch will close the meeting and will have some words of his own to add.

Chapter 4

REPORTS OF RAPPORTEURS

Item 1. L. E. Niemeyer and D. G. Fox, Meteorology Laboratory U.S. Environmental Protection Agency

Item 2. S. E. Larsen, Danish Atomic Energy Commission Research Establishment Risø

Item 3. P. M. Roth, Systems Applications, Inc., U.S.A.

Item 4. K. E. Grønskei, Norwegian Institute for Air Research

Item 5. F. B. Smith, British Meteorological Office

Item 6. B. A. Egan, Environmental Research and Technology, Inc., U.S.A.

5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

Item 1: Report of Rapporteurs - L. E. Niemeyer (U.S.A.)
and D. G. Fox (U.S.A.)

Modeler-User Workshop

The workshop period occupied all of the first day and also the morning of the second day of the 5th NATO/CCMS Panel Meeting, and the fact that some sixteen papers were presented (Chapters 5-20) left rather inadequate and uneven time for open discussion. Also, in contrast to the many modelers, there were actually very few users in attendance at the workshop and this restricted the input of user attitudes into the discussion. Under these circumstances no attempt has been made to provide an accurate account of all of the individual remarks, but rather only the rapporteurs' selection and general interpretation of significant major comments. Two extensive Canadian papers that were not presented at the meeting, because of the absence of their authors, are now included in the Proceedings as Chapters 21 and 22.

Jones (U.S.A.) emphasized on several occasions the urgent need to specify confidence limits for the pollution concentration estimates provided by air quality simulation models. Although this led to some lengthy discussions, no firm conclusions were reached and the question remains to be resolved. Milan (Spain) made the point that considerable subjective expert judgment was still required to correctly use air quality simulation models. Smith (U.K.) observed that the original Pasquill dispersion parameters that were utilized in many Gaussian-plume air quality models were intended for use in estimating the impact of great level sources, and were not intended to be used for elevated sources.

The problem of estimating sulphate emissions resulting from the use of catalytic converters on automobiles in the U.S.A. was described in a paper by Niemeyer (U.S.A.) [Chapter 16]. In response to a question by Jones (U.S.A.) it was agreed that in this case the choice of appropriate emission factors is the weakest link in the modeling exercise. Niemeyer indicated that emission factors were estimated from a small amount of test data collected by the EPA laboratories in Ann Arbor, Michigan, and that accurate data was very difficult to find. In regard to line-source highway modeling Mage (Denmark) referred to the effects of obliquity of the wind that was mentioned in the Turner Workbook. Calder (U.S.A.) said that he had discussed this matter further in a short paper in Atmospheric Environment. In further discussion of the paper on modeling pollution from highways, Fox (U.S.A.) mentioned that there are some questions regarding the use of Pasquill-Gifford dispersion parameters in the model, when calculating concentrations very close to the source. In the U.S.A. field experiments were being made that included the release of inert tracers from automobiles, and sampling of the tracer downwind of the highway. The data was being analyzed to give estimates of the σ's near the highway. Kropp (F.R.G.) stated that emission factors for mobile sources were given for CO, HC, SO_2, NO_x and Pb in the Köln emissions inventory that was presented at the 4th Meeting of the NATO/CCMS Panel, but Jones (U.S.A.) wondered whether the driving cycle was relevant to U.S. driving cycles. Kropp (F.R.G.) indicated that it was different from the U.S. California driving cycle, although similar to a European driving cycle.

A paper on episode planning was presented by Niemeyer (U.S.A.). Smith (U.K.) said that he would like to suggest on the basis of experiences in England that a useful addition might be to alert hospitals when an episode is expected. Slater (U.S.A.) said that he believed it was 5 or 6 years since the U.S.A. last had a serious air pollution episode and wondered where there was any reason to believe that the control required to meet the EPA ambient air quality standards had resulted in a reduction of air pollution episodes. Niemeyer (U.S.A.) thought that this might be possible although also believed that there had not been the necessary meteorological conditions. Clarenburg (Netherlands) observed that the measures seemed to have been designed for SO_2 and particulate pollution, and wondered about forecasting for photochemical pollutants 12 hours in advance. Simmons (U.S.A.) stated that photochemical pollution levels were now being forecast in California, although it was early to say whether the method was successful. Olsson (Sweden) indicated that in Sweden they had just begun forecasting the joint probability of occurrence of high pollution and precipitation, in an attempt to forecast the acidity of rainfall.

Item 2: Report of Rapporteur - S. E. Larsen (Denmark)

Development of a Common Data Base for Air Quality Modeling

See Chapter 23 [Considerations of the U. S. Regional Air Pollution Study - by D. G. Fox (U.S.A.)], Chapter 24 [A Common Data Base for Air Quality Modeling - by R. E. Ruff (U.S.A.)] and Chapter 25 [Verification of the Gaussian Plume Model - by L. E. Olsson (Sweden)]

In connection with the discussion of the U. S. Regional Air Pollution Study, Millan (Spain) enquired whether remote sensing techniques would be used in the validation of the air quality simulation models, and Fox (U.S.A.) indicated that remote sensing would only be used for meteorological measurements, e.g., the determination of mixing depths. In reply to a question as to what he believed to be the most important reason for the improved agreement that was claimed for complex models, Fox (U.S.A.) considered that this was due primarily to the utilization of the entire wind field rather than a single station observation. Mage (Denmark) pointed to the fact that air pollution measurements are frequently made at locations that are not typical for human population exposure, and said that a random sampling procedure should be adopted to avoid this problem. Clarenburg (Netherlands) asked whether model validation studies had been based on other pollutants besides SO_2, and whether validation for SO_2 would also imply validation for other pollutants. Fox (U.S.A.) indicated that validation had been attempted in modeling CO pollution, but that the most extensive validation data was for SO_2. Busch (Denmark) referred to the common data base requirements for air quality modeling and pointed to the difficulty of making different groups work together with one general data collection network. He enquired as to what strategy had been employed in deciding on data inputs and the basic types of analysis to be made on the data. Fox (U.S.A.) stated that for the U. S. Regional Air Pollution Study if a group wanted to use the information from the data bank, then they had themselves to supply input data in a prescribed format. Olsson (Sweden) described an attempt to apply and validate a Gaussian plume type model for Stockholm. He indicated, in reply to a question by Mage (Denmark) as to whether the correlation coefficients he had described showed any systematic variation with time, that this was indeed the case. Keddie (U.K.) asked whether the performance of the model was improved by calibrating it against observational data or by some other method. Olsson (Sweden) replied that it was done by generalizing the model. Calder (U.S.A.) regretted that with such limited time for discussion, it was unavoidable that many very important details had to be omitted, although these details would become quite critical if it was desired at some future time to standardize the models. Olsson (Sweden) mentioned that some details of the Stockholm model had been published in an article in the journal Atmospheric Environment. Busch (Denmark) said that it seemed to him that the model was being calibrated rather than validated, and enquired why spectral methods had not been used in the validation attempts, since these provided an efficient method for separating short-period and long-period variations. Olsson (Sweden) said that he thought that validation and calibration were simultaneously involved and that the suggestion to use spectral techniques might be a good one. Slater (U.S.A.) enquired how to determine if dispersion conditions are representative in a climatological sense. He stated that his group had been asked to analyze what effects the recent oil embargo might have had on the air pollution situation. In the U.S.A. there had been an unusually mild winter and it was not clear how to separate these two causes for the decrease in pollution concentrations. Olsson (Sweden) considered that a model, together with monitoring, might be able to handle extreme situations.

Item 3: Report of Rapporteur - P. M. Roth (U.S.A.)

Validation of Air Quality Simulation Models

See Chapter 26 [Validation and Sensitivity Analysis of the Gaussian Plume Multiple-Source Urban Diffusion Model - by R. C. Koch and S. D. Thayer (U.S.A.)] and Chapter 27 [Computing Optimal Air Pollution Abatement Strategies - by S. Gustafson (Sweden)]

Calder (U.S.A.) briefly referred to two papers on validation and sensitivity analysis for the Gaussian plume model, that had resulted from a contract let by the U.S. Environmental Protection Agency (see Chapter 26). His main desire was to draw attention to this work and indicate how a more detailed report could be obtained from the U. S. Department of Commerce by those who might be interested. This particular version of the Gaussian plume urban dispersion model contained a few novel features that he thought might be of interest to other modelers, including an approximate method for reducing the computation of two-dimensional integrals that are required to calculate concentrations from area-source emissions to one-dimensional integrals. This possibility considerably relieved the computational burden.

Gustafson (Sweden) presented a paper that described some numerical experiments with field data from Stockholm, relating to the computation of least-cost pollution abatement strategies. In answer to a query by

Fox (U.S.A.) as to what data was really needed to utilize the least-cost analysis, Gustafson said that information on concentrations and population statistics was required. Slater (U.S.A.) enquired how the cost functions were obtained and thought they would be very difficult to acquire. Moreover, there is more information on costs of control than on costs of damage and this could be dangerous politically. Grønskei (Norway) said that it was the intention to reduce the maximum concentrations, and enquired whether temporal control could be considered. Gustafson indicated that although this had not been done, it could be. Olsson (Sweden) said that he thought the method would be most useful in land-use planning in connection with urban dynamics models. Similar methods had already been used in connection with hospital planning.

Item 4. Report of Rapporteur - K. E. Grønskei (Norway)

Short-Term and Real-Time Modeling

See Chapter 28 [Modeling for Supplementary Control Systems - by B. A. Egan (U.S.A.)], Chapter 29 [On the Lognormal Distribution of Air Pollution Data - by D. T. Mage (Denmark)] and Chapter 30 [Statistical Description of Air Pollutant Concentration, Averaging Time and Frequency - by S. E. Larsen and E. L. Petersen (Denmark)]

Dr. Egan (U.S.A.) described a study on supplementary control systems made by Environmental Research and Technology, Inc. under a contract with the U. S. Environmental Protection Agency. This dynamic emission control system, which aimed at decreased pollution emission when meteorological conditions were unfavorable for dispersion, involved fuel switching, load shifting and temporary curtailment of emissions. The development of the supplementary control system required monitoring of ambient air quality, meteorological forecasting, emission forecasting and air quality modeling. Clarenburg (Netherlands) referred to work carried out in The Netherlands in 1968, on forecasting air pollution episodes, and that they had found good correlation between predicted and observed concentration values. Slater (U.S.A.) expressed his interest in the statistical use of the model calculations to design an optimum air quality monitoring system and enquired as to the criteria that were used to select the number and location of the monitoring stations. Egan (U.S.A.) indicated the need to locate and measure the peak values and the desirability for at least one monitoring station to be within 20% of the maximum value. The air quality model predictions were based on the spatial distribution of emissions and the frequency distribution in time of wind and atmospheric stability conditions. Based on the computed concentrations it was possible to rank the different possible locations for a monitoring station. Busch (Denmark) enquired as to what extent supplementary control systems were actually used. He indicated that in Denmark industry preference was for a simple permanent control rather than a complicated temporary one. Egan (U.S.A.) replied that the AIRMAP (Air Monitoring Analysis and Prediction) system developed by Environmental Research and Technology, Inc. had been in operation for some time. However, industry had not been required to reduce emissions based on a forecast. Only when an actual air pollution episode occurred had the emission reductions been required. More work was needed to determine the reliability and effectiveness of the temporary control system. Clarenburg (Netherlands) referred to five years of actual experience with a temporary emission reduction system based on their forecasting system and a voluntary cooperation by the industries in the Rijnmond area of The Netherlands.

The two papers that followed related to statistical aspects of air quality data. Professor Mage (Denmark) first considered the lognormal distribution of concentrations and suggested that a much better fit with observational data was obtained by assuming that a linear transform aX+b of the concentration X was lognormally distributed rather than X itself.

In his paper Dr. Søren Larsen (Denmark) showed the importance of spectra and correlation functions for the development of statistical models. He discussed the statistical model developed by Dr. Ralph Larsen in the U.S.A. and how this work might be extended in terms of power spectra, autocorrelation functions and consideration of running-mean values. He considered several sets of data and showed that a sum of two exponential functions closely approximated the autocorrelation function over a wide range of lag times. For lags less than one day a single exponential may suffice, with a time constant of about six hours.

In connection with these two contributions Slater (U.S.A.) referred to Ralph Larsen's work. The lognormal distribution may apply to data obtained from large cities, although it does not fit the distribution of ambient air concentration around a single large source. Also, it is difficult to describe the tail of the statistical distribution corresponding to the high concentrations that may occur 1-2% of the time. Clarenburg (Netherlands) observed that the measurements from a background station are usually not lognormally distributed. An exchange of viewpoints took place between Mage (Denmark) and Keddie (U.K.). Mage argued that the lognormal distribution could not be valid for a data set that included zero values. Keddie (U.K.) pointed out, however, that the ambient air concentration of a pollutant is never really zero. It is rather the lack of sensitivity of the measuring instrument that causes zero observations.

Item 5: Report of Rapporteur - F. B. Smith (U.K.)

Modeling of Complex Topographic Effects

See Chapter 31 [Fluid Modeling Program of the Meteorology Laboratory, U. S. Environmental Protection Agency - by W. H. Snyder (U.S.A.): presented by D. G. Fox (U.S.A.)] and Chapter 32 [A Quantitative Approach of Climatological Site Study - by J. P. Granier (France) et al]

a. Snyder's Paper

Keddie (U.K.) asked if water-channels have any value beyond flow visualization to which Fox (U.S.A.) replied that there were problems introduced by the limitation of scale imposed by the walls of the Channel. Olsson (Sweden) then asked about the use of stratified wind tunnels and what potential they had for studying realistic flow fields. Fox (U.S.A.) stated that some two or three existed around the world, but that an essential difficulty arises from the rather thin bounday layers that are generated. He reminded the meeting that one such study had been reported at the Charlottesville meeting in 1973. Barrett (U.K.) asked if the widths of wind tunnels were adequate for simulating horinzontal fluctuations to which Fox (U.S.A.) replied that since such fluctuations would be hard to model adequately the results could only refer to short-averaging times.

Grønskei (Norway) asked what scales within a city could be adequately simulated. Fox (U.S.A.) felt that a meaningful test would be to model different 1 x 1 km squares within St. Louis and study the differences in the turbulent fields resulting. To simulate the whole city with its heat island would be very difficult. Mery (France) stated that it was only possible to achieve simulation up to a real-life 10-minute time-scale in a wind tunnel (i.e., simulating small-scale turbulence) and to incorporate larger scales would require the additional involvement of numerical models. This was agreed and a brief discussion took place on the relation between the relevant length and time scales.

b. Granier's Paper

Smith (U.K.) referred to the modified curves showing the lateral angular spread σ_θ as a function of sampling time deduced for the proposed power station site and asked if there were any indications of an effect of topography (as wind direction changed) on these curves. Grainier replied that in the important wind directions no such effect was evident. However, in reply to Grønskei (Norway) he confirmed that the flow fields as indicated in their water-tunnel trials showed that topography did bend the trajectories and that such a behavior would be incorporated in their dispersion model.

To a question from Weber (F.R.G.), Mery (France) quoted an expected emission rate of 800 tons/day sulphur dioxide from the proposed power station.

Busch (Denmark) took up the important question of the relevance of the wind measurements on their 35-metre tower to the likely behavior of the chimney plume at several hundred metres. He noted that wind and turbulence could be radically different. Mery (France) pointed out that they were principally concerned with north winds (since these tended to be rather persistent and blew towards the local town of Arles), and with these the character of wind and turbulence tends to vary little with height. Busch (Denmark) also noted that at these heights the dispersion of the plume can be principally dominated by turbulence generated within the plume and not by the ambient turbulence.

Slater (U.S.A.) asked how the height of the stack was chosen. Mery (France) replied that although his group had some say the decision was actually that of a Government Committee.

Item 6: Report of Rapporteur - B. A. Egan (U.S.A.)

Recent Developments in Air Quality Modeling

See Chapter 33 [Research Program of Model Development Branch of EPA - by D. G. Fox (U.S.A.)], Chapter 34 [Assessment of the Validity of Airshed Models - by P. M. Roth (U.S.A.)], Chapter 35 [Empirical Approaches to Air Quality and Meteorological Modeling - by W. S. Meisel (U.S.A.)], Chapter 36 [Dispersion from Tall Stacks - by W. Klug (F.R.G.)], Chapter 37 [Some Views on Modeling Dispersion and Vertical Flux - by F. B. Smith (U.K.)]

In the first paper Fox (U.S.A.) briefly described some of the air quality modeling activities of the Model Development Branch of the United States Environmental Protection Agency. These activities consist of both "in-house" work, and sponsored research. A number of activities in the areas of boundary layer structure, surface energy structure, and dispersion climatology are associated with support of the RAPS study. Predictive wind flow pattern model development for urban areas and in complex terrain is being performed under contract research and would be expected to be continued in parallel and coordinated with wind tunnel modeling activities. Weber (F.R.G.) noted that the numerical model results illustrating the temperature field differences above some modeled one kilometer-wide urban green belts showed that the use of green belts produced only a minor local effect on the temperature field--a somewhat surprising result. Fox (U.S.A.) agreed noting that the model was only two dimensional, but that essentially no differences in the temperature fields were predicted beyond 50 to 100 meters above ground level. Grønskei (Norway) inquired about further information for the prediction of wind fields. Fox (U.S.A.) described two approaches being pursued--the first along the lines of Mr. Fosberg's work at the U.S. Forestry Service which utilizes an elliptical equation to predict stream functions from input surface temperature fields. The second approach uses potential flow theory and is to be applied for the complex terrain situation in the form of conventional boundary value problems.

Roth (U.S.A.) then presented a review of the types of photochemical modeling activities being performed in the U.S. In particular, Roth discussed the relative approaches and merits of "trajectory type" analyses vs the "grid point" models. He emphasized the need for good emissions inventory data on the various hydrocarbon species for input to realistic photochemical models. He then described a verification study performed to identify differences between the grid type numerical model predictions for an inert trace gas vs analytic solutions for some assumed power law variations of U(Z) and turbulent diffusivity K(Z). Results showed that:

(1) for the physical scales assumed, errors of less than 10% might be expected from the neglect of horizontal diffusion;

(2) the neglect of vertical motions may often be small but can, under conditions of convergence or divergence, given errors as large as 50%;

(3) the neglect of wind shear can result in errors as large as 50%;

(4) pseudo-diffusion errors associated with the present computational scheme can produce errors in the range of 10-20%.

Olsson (Sweden) inquired whether the three to eight minute vertical mixing time scale used by Roth was realistic. Roth (U.S.A.) thought it was. Busch (Denmark) commented that this order of magnitude was predicted by the numerical work of Deardorff under unstable conditions and that this estimate was also consistent with the observation that under unstable conditions potential temperature and some pollutant concentrations had a nearly constant value in the vertical within the planetary boundary layer up to a capping inversion height. These facts imply rapid vertical mixing. Roth (U.S.A.) commented that the higher concentrations of NO near the ground actually depletes the ozone concentration near the ground and a slightly positive vertical ozone gradient was often observed up to the capping inversion layer. Sholburg (Switzerland) inquired about the quality of information on chemical reaction rates relative to the uncertainity in meteorological inputs. Roth (U.S.A.) discussed the difficulties in attempting to verify laboratory data results under uncontrolled conditions in the atmosphere and pointed to even more severe validation problems when water droplets, heterogeneous reactions, etc. were involved.

Klug (F.R.G.) then presented a paper on the dispersion from tall stacks. Klug has been studying data received from the Tennessee Valley Authority on their Paradise steam plant operations. An extensive set of meteorological data, SO_2 monitoring data and emissions data was made available for this purpose. Klug presented preliminary results showing several areas of difference between observations and the results of dispersion estimates using conventional methodologies involving Pasquill/Turner stability classifications and dispersion coefficients. In the discussion period Klug described the specific changes which he felt would improve the methods for estimating dispersion. He felt that conventional methods would predict very unstable atmospheric conditions too often, leading to high estimates of concentrations at short distances. In addition, Klug felt that under high wind velocity conditions more stable atmospheric conditions actually existed than would be derived from the Pasquill/Turner criteria. Smith (U.K.) noted that the temperature differences from 1.5 meters to 100 meters which were used to determine atmospheric stability were susceptible to local ground surface conditions, as a result of the proximity to the ground of the lowest temperature measurement. Smith contended that the soil may respond differently in different seasons, and that a better measure of stability would be obtained if the lower temperature were higher, say at 10 meters above ground. Klug felt that no systematic errors would necessarily be introduced, but noted that his analysis was limited by data available from TVA. It was noted that the background levels of sulfur dioxide for this TVA data set are probably quite small. The data was collected in 1971. Salter (U.S.A.) felt that TVA would make this data more generally available if desired.

Smith (U.K.) then presented a discussion of limitations on dispersion prediction. Noting that errors in the horizontal and vertical dispersion coefficients over uniform terrain could be expected to be no less than 10-15%, Smith pointed out that the expected error in the location of the maximum concentration downwind of an elevated point source could have an accuracy no better than 35%, and that the value of the maximum concentration has an error range of over 50%. Furthermore, if one takes into account uncertainties regarding whether the wind direction was directly from the source to receptor, errors of over 100% could be expected at any fixed point. Smith noted that if surface roughness or other terrain inhomogenieties were taken into account, simple relations between concentrations and dispersion estimates do not hold, and that one is led to approach the problem with the conservation equations. Smith then presented equations describing the diffusion of emissions from a line source near the ground in terms of second order turbulence statistics. Smith noted that the estimate of rate of change with time of the vertical flux of pollutant material would require knowledge of the turbulence statistics to accuracies of 1 part in 100. This problem arises essentially from the need to estimate the vertical flux rate from differences between large numbers.

In the ensuing discussion, Barrett (U.K.), Busch (Denmark), Fox (U.S.A.), Egan (U.S.A.) and Slater (U.S.A.) inquired about how to get around this problem and expressed concern over the pessimistic warning of Smith's presentation on the general question of how useful advanced models would be to future applications. Barrett wondered whether the same conclusions would be reached from alternative formulations of the conservation equations which perhaps did not focus on the time rate of change of elements.

Fox (U.S.A.) expressed the view that the second order closure modeling has been studied in more detail than Smith had implied. In particular, Fox noted that Donaldson of U.S.A. has investigated these methods with respect to wind tunnel flow measurements, and that Lumley had put these closure methods on a firm theoretical foundation. Smith maintained that when one goes to the more complex equations, one needs very accurate meteorological data, and noted that unless very accurate data was obtained, improvements over simpler closure schemes, such as gradient transport of "K" theory, might be minimal.

Chapter 5

INTRODUCTORY REMARKS

by

Kay H. Jones
U. S. Environmental Protection Agency

5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

Introductory Remarks

by
Dr. Kay H. Jones
Air Pollution Pilot Study Director

This Modeling Panel Meeting represents the last formal activity to be sponsored under the auspices of the Air Pollution Pilot Study except for the ongoing and continuing cooperation on the Low Pollution Power Systems Development (LPPSD) initiative. The Pilot Study, which was introduced at the inaugural plenary session of CCMS, was culminated with the submission and adoption of a final report containing fifteen far-reaching action recommendations at the plenary session held on May 7-8, in Turin, Italy. I can say without reservation that the Pilot Study accomplished all of the objectives which were set forth in the original study proposal. The timeliness and effectiveness of the Air Pollution Pilot Study epitomized the unique CCMS approach to solving major environmental problems common to the NATO community.

I think it would be appropriate to review briefly the fifteen recommendations which were derived from the study in that several of them relate to historic and most successful activities of this panel. These recommendations are:

RECOMMENDATION I

Member nations will assess the air pollution in cities of 100,000 inhabitants or greater and industrial areas within their national boundaries. Member nations should establish such assessments by 1980.

- RECOMMENDATION II

  Member nations will establish effective air quality monitoring systems including the measurement of meteorological parameters.

- RECOMMENDATION III

  Member nations will employ reference methods endorsed by the World Health Organization (WHO), the Organization for Economic Cooperation and Development (OECD), and/or the International Standards Organization (ISO), or alternatively methods which have been shown to be comparable to these reference methods.

- RECOMMENDATION IV

  Member nations will establish systems for monitoring data storage and retrieval such as those employed by the WHO.

- RECOMMENDATION V

  Member nations will conduct emissions inventories employing the uniform procedures, where applicable, based on the experience derived from the CCMS assessment studies.

- RECOMMENDATION VI

  Member nations will cooperate to develop standardized methods for emissions data storage and retrieval to support requirements in the conduct of national air quality management programs. The U.S. National Emission Data System (NEDS) might serve as a model for a common international system.

- RECOMMENDATION VII

  Member nations will cooperate to develop standardized techniques for projecting emissions and predicting future ambient air quality.

- RECOMMENDATION VIII

  Member nations, in accordance with national priorities, will set ambient air quality standards or objectives. The CCMS criteria documents and the criteria and guides developed by the WHO should be used in this process.

- RECOMMENDATION IX

  Member nations will participate in the WHO program for development of criteria documents as well as in the revision of existing criteria documents.

- RECOMMENDATION X

  Member nations will support strong national research programs and cooperate internationally for the purpose of developing additional criteria on the environmental effects of all air pollutants.

- RECOMMENDATION XI

  Member nations will use, inter alia, CCMS control technology documents in developing plans for applying controls to existing pollution sources to improve air quality.

- RECOMMENDATION XII

  Member nations will, in the course of industrial expansion, employ the best available and practicable control technology on an industry-by-industry basis.

- RECOMMENDATION XIII

  Member nations will assure the exchange of new information on research, development, and demonstration of the control technology. CCMS derived control technology documents should be updated periodically to reflect significant advances. The appropriate international body for this effort is the WHO International Reference Center for Air Pollution Control.

- RECOMMENDATION XIV

  Member nations agree the CCMS modeling activity has shown that there is a widespread need for further international cooperation to accomplish the following tasks:

  - Continue to bring together model developers and air quality managers for exchange of ideas, discussion of users needs and demonstration of modeling techniques.
  - Standardize modeling techniques for specific air quality management applications, as well as give consideration to methods for efficient dissemination of such models to all users.
  - Continue to review on-going air quality assessment studies.

- RECOMMENDATION XV

  Participating nations agree to take necessary actions to implement fully the LPPSD Memorandum of Understanding, with emphasis on collaboration on the total systems approach for developing environmentally compatible motor vehicles taking into account air quality, safety, energy, and noise.

As you can see, Recommendation XIV clearly recognizes the desirability to continue and broaden the Modeling Panel's activity. In this regard the Federal Republic of Germany is planning to introduce a new initiative at the October plenary setting forth such a program. The U.S. has stated its intention to co-pilot this undertaking and many other delegations at the Turin meeting emphasized their interest and intent to participate in such an initiative. In addition to the modeling aspects of the new program, attention will also be given to Recommendations V, VI, and VII for improvement and standardization of emissions inventory techniques as well as continuing a forum to discuss city-by-city assessment study results.

The first day and a half of this meeting, as you know, is being devoted to a workshop where modelers and users are being brought together for the purpose of closing the communication gap which was discussed by myself and others at last year's meeting in Oberursel. If you will recall, I stated that such modeler/user workshops could serve to overcome the following problems:

(1) Many modelers wish to look upon their work as a continuing scientific research endeavor, rather than developing a dynamic tool for application in air quality management programs.

(2) The antithesis of (1) often occurs when users employ the results without the confidence limits to reach very tenuous decisions.

(3) Users at the policy decision level normally do not have the slightest working knowledge of modeling, and hence lack confidence in the output product when arguing in the political arena.

(4) Air pollution modelers should make inputs in the data analysis for all types of air quality modeling, even though the meteorological factors are not explicit variables in the model, e.g., rollback modeling.

(5) Users have little appreciation for the research costs for improving the atmospheric modeling science.

It is premature to predict the relative success of this first workshop, however, the mere holding of such a forum is probably the greatest hurdle we have overcome in attempting to close such an obvious chasm in communications between the scientific and policy levels in a critical environmental problem area.

The beautiful environment of Denmark and the excellent program established by our Danish hosts for this meeting are most conducive to the success of this Modeling Panel meeting and as the Pilot Country we extend our sincere gratitude for their invitation.

Chapter 6

MISCELLANEOUS QUESTIONS RELATING TO THE USE OF AIR QUALITY SIMULATION MODELS

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

I. Introduction

Last year's workshop discussion of modeling and users' needs brought out a number of important questions. Indeed it provided the primary stimulus for the user-modeler interface workshop now being held at our 5th Meeting, and which aims at improving the communications between the potential users and developers of air quality simulation models. As a basis for continuing the discussion the present paper attempts to recapitulate some of the more critical questions raised at the earlier meeting and to develop a few additional ones that have occurred to the author from time to time. Very little novelty is claimed although almost certainly others would give some different emphasis. In any case the author must be held solely responsible for any misinterpretations of attitude or departures from the views that may be held by his collective colleagues in the modeling community. At least it is hoped that any differences will serve to stimulate future discussion.

II. The critical property of air quality simulation models (AQSM's) for air quality management

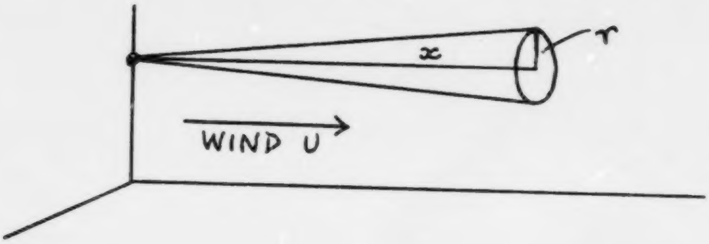
If one accepts the overall philosophy of ambient air quality standards, then the simplest means of achieving these standards when they are presently exceeded is the so-called proportional or rollback method. In this it is assumed that, all other things being the same, if every source of pollutant is reduced by the same factor then the total concentration at all receptors will be reduced by the same factor. For non-reactive stable pollutants this will follow from the facts that, firstly, the pollutant concentration produced at a receptor location by each individual source is directly proportional to the source emissions rate (This is so for zero background concentration; otherwise, the concentration excess over the background value needs to be considered). Secondly, the total concentration at the receptor resulting from the simultaneous emission from all the sources is the arithmetic sum of the individual contributions (or individual excess values if the background is not zero).

The serious shortcoming of this simple rollback model is that it is only concerned with the integrated effect on air quality of all the pollution sources that are present. It is not concerned at all with the relative concentration contributions from the individual sources. For example, even if the air quality at some receptor location is dominated by the contribution from a nearby source of small magnitude, the proportional reduction formula will still call for the same proportional reduction of emissions from a possibly non-contributing distant source as it does for the dominant nearby small source. This would certainly appear to be an unacceptable basis for air quality control as it would, in principle, require control of non-contributing sources. Evidently, what is needed is some method by which the relative magnitudes of the concentration contributions from the different sources can be estimated, and particularly if a cost-effectiveness approach to pollution control is to be adopted. This is exactly the purpose of the AQSM. The latter aims to calculate the spatio-temporal distribution of air pollution concentrations that would occur under some specified meteorological conditions (these influence the atmospheric transport and dispersion of pollutants), and for any specified but arbitrary distribution of pollutant emissions. Thus the AQSM will allow quantitative estimates to be made of the significance, for air quality, of the different pollution sources within an area, and will thus provide a rational basis for the control of the individual sources.

III. A simple example of a model for atmospheric dispersion

What at first sight might appear to be one of the more difficult problems involved in developing an AQSM, is the need to estimate the atmospheric transport and dispersion of pollutant in its passage from the source to a receptor, i.e., so that the ambient air concentrations can be calculated in terms of the rates of emission. From a fundamental physical point of view this is a very complicated problem of atmospheric fluid dynamics. However, useful practical solutions can be obtained. It may be of interest to non-modelers to show in a simple fashion how this can be done, by considering a model for atmospheric dispersion from a continuously emitting point source. Although, thanks to our air pollution control activities, this is no longer a common sight, there will be few of us who have not at some time watched the spread of a smoke plume from a tall chimney stack. Under conditions of moderately strong winds and of cloudy skies, the smoke plume travels out horizontally and appears very roughly as a rather narrow cone of material, with apex at the source.

As a basis for a very simple dispersion model we will assume this to be the case as shown in the diagram below. Here r is the radius of the cross-section at downwind distance x, and for simplicity we shall assume a uniform distribution of concentration in any cross-section.



We shall also assume that $r = ax$, where a is a constant to be specified, and denote the wind speed by U. As the plume slowly expands, with increasing distance from the source, the smoke concentration will diminish. If Q (g/sec) denotes the steady rate of release from the continuous point source then, if the smoke material is conserved, this must equal the rate of transfer of matter through any cross-section downwind, i.e., a circle of area πr^2. Thus, if C_p denotes the concentration in the cross-section at distance

$$Q = \pi r^2 \times U \times C_p$$

or

$$C_p = \frac{Q}{\pi U r^2} = \frac{Q}{\pi U a^2 x^2} \qquad -(1)$$

Although somewhat artificial we may also consider the concentration, say C_L, downwind of an elevated crosswind line source of pollution of unlimited extent. If q is the rate of emission per unit length of the line source (g/cm/sec), then it follows very simply from equation (1) that

$$C_L = \left(\frac{q}{\pi U r^2}\right) \times 2r = \frac{2q}{\pi U a x} \qquad \text{— (2)}$$

If, instead of being elevated, the point source emission had been at ground level, then we will assume that the plume would have been a half-cone rather than a complete one, so that the concentration would be double that given by equation (1). Similarly, of course, for an extended line source at ground level the concentration would be double that of equation (2). To evaluate these formulae it will be necessary to assign a value to the constant a, which expresses in the crude model the rate of dispersion of the material. Although, in general, this will be a function of the meteorological conditions, for cloudy skies and moderate winds visual observation of smoke plumes shows that it is reasonable to take $a = \frac{1}{10}$ (corresponding to an angle of spread for the elevated conical plume slightly greater than 10°. We now compare the predictions of the simple formulae (1) and (2) (actually as amended for sources at ground level) with the classical observational data established by Sutton (Micrometeorology, McGraw Hill Book Co., 1953), for clouds of smoke and gas traveling over open level downland and under conditions of small vertical temperature gradient. We find:

(i) Observations show that the concentrations from a steady continuous emission vary directly as the source strength, in agreement with equations (1) and (2).

(ii) Observations show that concentrations vary approximately inversely as the mean wind speed, in agreement with the model equations.

(iii) Observations show that the average height and width of a cloud vary little with wind speed. This is consistent with a constant value for a in the above equations.

(iv) For $Q = 1$ g/sec, $U = 5$m/sec and $x = 100$m, diffusion experiments give $C_p = 2$mg/m^3 (actually the peak concentration) as compared with $C_p = 1.27$mg/m^3 for the model. Also, the concentration is found to vary like $x^{-1.8}$ as compared with $x^{-2.0}$ for the model.

(v) For $q = 1$g/cm/sec, $U = 5$m/sec and $x = 100$m, experiments give $C_L = 3500$mg/m^3 compared with $C_L = 2540$mg/m^3 from the model. Also, the line source concentration is found to vary like $x^{-0.9}$ as compared with $x^{-1.0}$ for the model.

(vi) An appropriately defined observed height and width of a point source cloud at 100m downwind are 10m and 35m respectively, which are close to the values of 10m and 20m respectively, for the simple half-cone plume above.

We thus see that, in spite of its extreme simplicity, the conical plume model is in close agreement with a considerable variety of field observations (an even closer agreement would be obtained by using a slightly different value for the constant $\underline{a} = \frac{1}{13} = 0.077$, which for ground located sources gives $C_p = 2.15$mg/m^3 and $C_L = 3310$mg/m^3). If a general moral can be drawn from this simple example it might be that, although available models may frequently be far from perfect, they may still give far better estimates of air quality than could be obtained by any other method.

The simple model above is in basic principle quite similar to the general system originally proposed by Dr. F. Pasquill in 1961 (see Atmospheric Diffusion, by F. Pasquill, D. Van Nostrand Co Ltd, 1962). This provides approximate estimates of diffusion which, in a very slightly modified form, have been the basis ever since of the so-called Gaussian plume models of dispersion in AQSM's. Instead of a uniform concentration distribution in each cross-section of a conical plume, as above, Pasquill considers the more realistic bell-shaped Gaussian distribution, in both the vertical and horizontal directions. He then proceeds to express these plume dimensions in terms of an angular crosswind spread and a vertical (height) spread. This serves to emphasize properties of the plume that are easily visualized and are part of even rather casual observational experience of plume behavior. In this respect the Pasquill Gaussian plume model has a strong advantage and special position relative to other more sophisticated approaches to diffusion modeling, such as by use of complex differential equations for atmospheric transport and diffusion. All of these approaches, like the Gaussian plume itself, are, of course, only mathematical expressions for the fundamental physical constraint of the conservation of matter.

However, the Gaussian plume expresses this conservation condition in terms that are directly related to normal observational or simple visual experience, while the inputs and properties of the eddy diffusion equations are elusive and beyond the reach of immediate experience.

IV. The high decision-value of AQSM's and the proper requirement for comprehensive verification studies

Because an AQSM provides the causal link between air quality and the sources of pollution, and one that is critical in any systems analysis approach to air pollution control, the present day requirements for modeling activity are legion. Other speakers will illustrate the variety of current uses of AQSM's and we shall here only emphasize the fact that extremely far-reaching decisions are now being based on modeling. Also, in many cases it would seem to be the only rational technique that is available. In the U.S.A., quite apart from the well-known use of AQSM's in the development of implementation plans and pollution control strategies, other more recent considerations of very far-reaching importance include such things as land-use planning, the location of new fossil-fuel burning power plants, the assessment of fuel substitution strategies such as the redistribution of sulfur-containing fossil fuels between power plants so as to minimize undesirable environmental effects, real-time alert warning systems, and real-time source emission control systems based on model estimates of air quality using forecast meteorological conditions.

It is evident that in all these considerations the decision-value of the AQSM is extraordinarily high, since the final action will in every case be a very major one. This in itself would seem to provide ample justification for much increasing the expenditures to develop improved AQSM's and to perform comprehensive verification studies so as to maximize confidence in the decisions and actions that will follow. However, in many cases it is only too common to find that there are very strong and urgent pressures to provide modeling results even when the model verification information may be quite marginal. There is frequently a strong tendency to push on too rapidly with rather formal theoretical extensions of modeling techniques that lack adequate experimental checks in the real atmosphere. In this connection it seems that we might do well to follow the example of Professor M.E. Berlyand's well-known air pollution modeling group at the Main Geophysical Observatory, Leningrad, U.S.S.R. In a recent book by Berlyand (Air Pollution and Atmospheric Diffusion, John Wiley & Sons, 1973) many field expeditions are described that have been undertaken by his group to obtain experimental corroboration of the theoretical formulae. These expeditions cover a wide variety of pollutants and industries, and indicate a deep concern with field validation of the theoretical predictions. Research expenditures for improved modeling capability should properly reflect the extraordinarily high decision-value of AQSM's. It seems that at the present time this is hardly so and in some situations it might be very disquieting if it were more generally appreciated that so much is really based on so little. This comment is certainly not intended to discourage the application of modeling, but only to suggest that the current uses of AQSM's are so critical that a greater dedication of resources for modeling seems to be amply justified.

Another aspect of this question that is apparent in the U.S.A. arises from the fact that the Environmental Protection Agency not only supports a major research and development program for AQSM's, but is also primarily responsible for law enforcement in all matters relating to environmental pollution and, in particular, the achievement of national ambient air quality standards. Where EPA decisions that are based on the use of AQSM's are unfavorable and conflict with the special interests of industrial polluters, strong efforts may be taken by industry to publicly discredit and question the decision through any weak features that can be exposed in the AQSM. This is frequently done by the hiring of expert modeling consultants. In this case it is obvious that the AQSM's that are used as a basis for decision must be capable of withstanding very close and frequently hostile technical scrutiny. This will only be possible provided that extensive verification studies have been performed.

(V) The modular structure of AQSM's and their validation

As first emplicitly emphasized by Dr. W. B. Johnson at our 3rd Meeting, most of the efforts to date at the validation of AQSM's have been confined to comparisons of the model calculations with observed air pollution concentrations. However, as was pointed out, this procedure is little more than a crude calibration and does not provide any clear cut information as to the parts of the model that may be in error. As Dr. F. Pasquill epitomized:

"Calibration may be consoling
But is a practice we shouldn't condone,
And for validation to have a virtue
The physics and chemistry must be known."

The AQSM is not simply an atmospheric dispersion model, of which a very simple example was given earlier. Rather is it a composite of many elements or sub-models, e.g., for the emissions of pollution, for atmospheric transport and dispersion, and for the physical and chemical transformations and removal processes. For time-dependent models -- like those of primary interest for photochemical pollution -- it is also necessary to consider the very difficult problem of specifying the initial three-dimensional distribution of several primary reactive pollutants, as this can have a major effect. To establish any high degree of overall confidence in the model, it is necessary to evaluate the individual elements and to make a sensitivity analysis to determine the overall sensitivity of the AQSM to variations of the inputs and to possible errors in the various sub-models. Through such sensitivity tests it is possible to delineate the scope and direction of field programs to determine air quality distributions, meteorological factors and distributions of emissions. Most available data sets for model validation studies are quite deficient in one respect or another, and typically the rather extensive volumes of data that have been compiled in the past show little attention for the specific requirements of the modelers. This was a primary reason in the U.S.A. for the extensive multi-year Regional Air Pollution Study (RAPS) now being undertaken in the St. Louis area, and which has been described at several of our previous meetings.

As the validation of AQSM's is a special discussion topic, for the third time on our agenda, this matter will not be pursued further in this paper. However, it may be worth mentioning, and particularly as the development of AQSM's has frequently been the purview of diffusion meteorologists, that there are already strong indications (as might have been expected) that one of the major sources of error in AQSM's stems from errors in the estimation of emissions distributions. In fact, it is my understanding that Dr. F. Gifford has recently shown that, for urban CO modeling, the use of a more sophisticated and accurate specification of emissions gives a significantly improved agreement with observed concentrations. This improvement is obtained even with great simplification of the meteorological-transport module of the model.

VI. Need for critical examination of the precise requirements for air quality inputs in a systems approach

The need for improved communications between the developers of AQSM's and the users of the models, such as the air quality management decision makers, has already been emphasized and is a prime subject for further discussion at this 5th Meeting. Not so frequently alluded to is the need also for improved communications between the developers of AQSM's and those, in a more comprehensive systems approach, having concern with the critical link between various levels of concentration and the effects of the pollution. Although very difficult, this vital question has only received rather superficial examination. However, its resolution is evidently necessary in order to provide a rational basis for specification of the accuracy required of air quality estimates using AQSM's. Since there is a multiplicity of model applications it may be expected that the accuracy requirements will be a function of the specific application, and that in some cases even crude estimates by AQSM's may be sufficient within a larger modeling framework. What is suggested is that just as the AQSM itself contains several distinct modules, as was emphasized in a previous section, so the entire AQSM is only a module in a more comprehensive modeling scheme that will involve air pollution damage functions, or perhaps economic considerations, etc. as well. A need exists for an analysis of the sensitivity of the output of the overall systems analysis model to variations in the AQSM input. In relation to the final output there has so far been little analysis of the question of how good the AQSM input needs to be. A large part of the problem is the imperfect knowledge at the present time regarding health effects and damage functions for air pollutants. Thus, present ambient air quality standards are expressed in terms of pollutant concentrations that are averaged over either 1 hour, 3 hours, 8 hours, 24 hours or the whole year, and in order to meet the air quality standard the appropriate actual concentration value must not exceed a specified standard value more than once per year. For all of the shorter averaging times this will involve the difficult problems of "rare" events that, in terms of the frequency or probability distribution of the concentration values, occur in the tails of the probability distribution rather than in its central portions. As is well-known, the tails of any distribution are extremely difficult to determine with any precision. Thus, in the case of air quality estimates based on an AQSM with a meteorological input to determine short-term average concentration values, it would be necessary to have an extremely long period of meteorological observations to be confident that some standard value would not be exceeded more frequently than once a year. Also, because of shifts in population and also ongoing pollution control programs, the distribution function is not likely to be stationary over a sufficient time to obtain a valid sample. Thus, the use of air quality standards that involve consideration of rare events can only lead to results of low statistical significance. To avoid some of these problems it seems desirable to improve communications between the developers of AQSM's and those concerned with quantification of the effects of air pollution. Improved statistical significance for the prediction of effects will require consideration of other than rare events, e.g., short-term averaged concentration standards that may be exceeded twice a year, three times a year, etc. This would require a generalization of the air standards in terms of statistical distributions.

VII. Recognition of the limitations of AQSM's

Reasonable agreement has been obtained between the predicted and observed concentration values in a number of applications of AQSM's. However, in view of the somewhat tenuous nature of the physical basis of many of these models, it is important to bear in mind that they need to be applied with proper caution and preferably by professional modelers, who will be most familiar with their limitations. This point has been emphasized very strongly, in a slightly different connection, by Professor R. S. Scorer ("Air Pollution," Pergamon Press, 1968) who says, "There are NO universal formulae which can be used to describe what will happen to pollution emitted into the air, and this needs to be said because formulae have been so misused in the past by people who have been secretly frightened of realities and have dispensed according to the prescription of the most fashionable wizard." Scorer points out that, because of the multitude of complexities that are the essence of many practical situations, such as topography, wind fluctuations and the diurnal variation of meteorological conditions, there is always a need to consider the ideosyncrasies of particular situations and this can only be done on the basis of an understanding of the basic mechanics and physics. This should be taken as a strong and authoritative warning against the rather frequently encountered temptation to use an AQSM at any costs and sometimes without proper regard for the realities of the actual situation

As we have seen previously, there are some situations for which even a very simple atmospheric dispersion model may be surprisingly good and yield very useful results. However, success in one problem area will not automatically imply success in others. As an example, most existing AQSM's are a lot less reliable in producing short-term real-time concentration estimates than they are in giving frequency statistics of these concentrations or long-term average values, such as would be of concern for the chronic health effects of regional air pollution. As was emphasized at last year's meeting, there is an ever present need for a clear statement of the limitations of any particular AQSM application. Attempts should be made, much more strongly than in the past, to place confidence limits on the model predictions and this will probably necessitate an expanded program of ad hoc experimental studies. It also seems most desirable that users be clearly and unequivocally informed of the current non-availability of validated AQSM's for a number of situations that are of potential interest such as for complex terrain, stagnation conditions and photochemical air pollution. This realization will hopefully stimulate increased allocation of resources for the development and improvement of AQSM's. In spite of some wishful thinking to the contrary, it is also necessary to recognize that there are some situations for which the physical conditions are so complex that, in all probability, modeling will not be adequate at any time in the foreseeable future.

Another circumstance, which may be worth a comment, and which may contribute to some loss of confidence in AQSM's among users, is the apparent wide choice of models that are available for application. Fortunately, this multiplicity is often quite illusory since in many cases we have only special-purpose minor variants of a single basic model, such as the steady-state Gaussian-plume dispersion model. User confidence might be increased if this fact were more frequently emphasized and a stronger effort made by the modelers to standardize the basic models that are now in fairly common use. This should, of course, follow a clear demonstration of the relative values of the various model types. At the same time there is a strong need to anticipate future needs and now that the general characteristics of an AQSM are very widely appreciated it would be helpful to modelers to know what additional types of applications the users may be visualizing or desiring.

VIII. Conclusions

The critical property of the AQSM for air quality management is the fact that it provides the quantitative causal link between air quality and pollution emissions. In principle it thus allows estimates to be made of the relative contributions of the various individual sources of pollution to the total pollution concentration at any receptor location. It thus provides a rational basis for the control of individual sources, in contrast to control by so-called proportional reduction or rollback.

The overall AQSM is a composite of many elements or sub-models, such as those for the spatio-temporal distribution of emissions, for atmospheric transport and dispersion, and for physical and chemical transformation and removal processes. To establish any high degree of overall confidence in the model, it is necessary to evaluate the individual elements and make a sensitivity analysis to determine the overall sensitivity of the AQSM output to variations of the inputs and to possible errors in the various sub-models.

The atmospheric dispersion sub-model is one of the most critical in any AQSM, although empirically-based models have now been successfully used for some time. These are based on direct measurements and observations of transport and diffusion as a function of meteorological conditions. Even very simple considerations may be useful in this connection, in order to codify approximately the results of observational experience.

At the present time very far-reaching decisions are based on modeling, and for many problems it would seem to be the only rational technique that is available. Typical examples relate to such things as land-use planning, the location of large power plants, the assessment of fossil-fuel substitution strategies, real-time source emission control strategies, etc. In such applications the decision-value of the AQSM is extremely high and, in consequence, pressures are frequently very strong to provide modeling results even when the model verification information may be quite marginal. Research expenditures and allocation of resources for improving modeling capability should more adequately reflect the critical decision-value of the AQSM at the present time. This need is further emphasized by the fact that the predictions based on the use of AQSM's will be subject to extremely close technical scrutiny whenever they lead to decisions and actions that may be unfavorable or conflict with the special interests of industrial operations. In the latter case there will be a strong temptation to discredit the adequacy of the AQSM, unless this is on a very firm foundation.

The need for improved communications between the developers of AQSM's and the users, such as the air quality management decision makers, has already been strongly emphasized and is under further discussion at this 5th Meeting. However, there is also a need for improved communications between the developers of AQSM's and those, who, in a more comprehensive systems approach, have concern with the critical link between air quality and the effects of pollution. This is necessary if only to define more adequately the accuracy requirements for air quality estimates using AQSM's. The problem is also noted of the low statistical confidence of predictions that involve consideration of "rare" events, e.g., that a certain short-period concentration value should not exceed a specified value more than once a year.

A warning is sounded against the frequent temptation to use an AQSM at any cost, and sometimes without proper regard for the realities of the actual situation. The need for a clear statement of the limitations in any particular AQSM application is noted, and once again the desirability is emphasized of attempting to place confidence limits on the air quality predictions of AQSM's. This will probably need an expanded program of specially designed experimental field studies.

The apparent multiplicity of models that are available for some applications, and which could possibly undermine a potential user's confidence, is in many cases illusory. This is because of the existence of many special-purpose variants of a single basic model, such as the Gaussian plume dispersion model. Stronger efforts should be made to standardize and document some of the more basic models that are now in fairly common use. The identification of additional types of applications of AQSM's, that are now visualized by the users, would be helpful to the modelers.

Chapter 7

POTENTIAL APPLICATIONS OF MATHEMATICAL-METEOROLOGICAL DIFFUSION MODELS TO THE SOLUTION OF PROBLEMS OF AIR QUALITY MAINTENANCE

by

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POTENTIAL APPLICATIONS OF MATHEMATICAL-METEOROLOGICAL DIFFUSION MODELS TO THE SOLUTION OF PROBLEMS OF AIR QUALITY MAINTENANCE

[Anwendungsmöglichkeiten von mathematisch-meteorologischen
Diffusionsmodellen zur Lösung von Fragen der Luftreinhaltung]

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FOREWORD

Maintenance of air quality is certainly of central importance among concerns in the area of environmental protection. Here, we are attempting to eliminate existing unacceptable immission conditions by improvement measures and, further, to take into account, through a reasonable, immission-oriented planning strategy, the fact of progressive increase in the density of population and of industrialization. The basis for all planning of this type is a prediction of future immission conditions. This prediction of the air quality as the result of predictions or plans in relation to emissions may be the most important current problem in the field of air quality maintenance.

We can extrapolate measured immission conditions from the past and present into the future only very uncertainly and without any great predictive power. Because of the complexity of conditions, the relation between cause (changes of emissions) and effect (changes of the air quality) cannot be determined from measurements alone. The mathematical-physical prediction on the basis of simulation models for the course of natural phenomena, which has been so successful in physics, appears to be a suitable aid for solution of the prediction problem.

The following discussions should justify this method of model simulations. In view of the difficulties in developing models, the basic possibility of solving immission-oriented planning problems with this method has often been questioned; but,these reservations must be discarded, because even today the results of model simulations of immission situations must be taken quite seriously as aids to planning strategy in the field of air quality maintenance. Much research is being done on this sector in all industrial nations, with the goal of developing better and better simulation models for the spread and transport of air pollutants in the atmosphere.

H. Fortak.

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INTRODUCTION

Air pollution is now present almost daily for the population in congested areas. The sources of man-made air pollution grow in intensity and spatial extent as a result of advancing urbanization, industrialization, and technology more and more. We can already perceive that air pollution will take on global dimensions by the end of this century. At the beginning of this century, the problem was small-scale and local. Measures for maintenance of air quality were necessary only in special cases, and were then done on the basis of legal regulations. In city planning, rude beginnings were made on influencing the build-up of industry on the basis of simple wind direction statistics so that, for example, there was a tendency in Central Europe to distribute industrial regions on the eastern boundaries of the cities. Economic, transportation, and often even sociological reasons, as well as the fact that many cities are now growing together into population centers, require city and regional planning measures of far more complex nature than was the case previously. It is apparent, for instance, that simple wind direction statistics alone will no longer suffice, because there are already very distinct differences in wind direction distribution from place to place inside the great population centers which take on dimensions of the magnitude of 10,000 km^2 and more. The existence of such great population centers makes it quite probable that changes in the radiation conditions can produce climatic changes. We have no knowledge of whether these will cause further deterioration in living conditions or not. Air pollution from human activities, then, represents a danger of hardly imaginable extent, a danger which can perhaps still be avoided by immediate planning measures in all industrial nations.

Conceivable measures are technological, on one hand, and legal, on the other hand. Limitation of the emission of harmful air pollutants with growing industrialization and technology through purely technological measures and developments represents the most plausible, if not the cheapest solution to the problem. Unfortunately, though, it appears today that technical advance in the field of dust removal and chemical purification of emitted gases will not win the race with the steady increase in the emission of harmful gases due to industrialization and increased technology. We can even calculate a doubling of the amount of air-polluting substances in the course of the next 20 years in spite of all technical measures. But the lawmakers, too, who are responsible for reasonable plans in the interest of all in the area of air quality maintance will demand too much in their measures, in view of the political consequences, particularly if these measures rest on scientifically contestable statements.

Aside from conceivable climatic changes as the result of growing air pollution, the capability of the atmosphere to distribute foreign materials from spatially limited materials both horizontally and vertically is quite astoundingly large. Because of this property of the atmosphere, immissions dangerous to humans occur relatively rarely, even in the vicinity of sources of very intense emissions. In many cases, large amounts of pollutants are carried to high altitudes so rapidly, due to special meteorological conditions, that only very slight immission values are found near the ground. From this there follows another possible measure for maintaining immission limiting values everywhere and at all times within industrial and urbanized areas of congestion. In cooperation with medicine and biology, the legislature establishes immission limits for all harmful materials as determined by technologists. Technologists, in cooperation with state authorities, make up a register of all emissions and make predictions of all the short-duration and long-duration emissions to be expected. On the basis of the emission register and the variability it shows in the spreading conditions, meteorologists make predictions of the immission conditions and establish when and where the prescribed immission limits will under certain circumstances be exceeded. Here planning experts come into action. Taking into consideration economic viewpoints, among others, they work out a strategy of partial emission reduction so that overstepping of the immission limits is prevented at the minimum cost. In this way, optimum use is made of the capability of the atmosphere to "dilute" harmful materials introduced to it very effectively so that the immissions at the ground remain relatively small.

A logical air pollution control strategy cannot appear other than described above. Fundamentally specified immission limits allow the introduction of control measures only for the predicted immissions; but, for these we have an unconditional need for knowledge about the emission register, and also knowledge of the meteorological process of transport and of the "dilution" from admixtures of air. The situation here is like that for almost all problems in physics. We study the time changes of a physical system starting from an initial condition if this system is exposed to time-variable external influences. In this case, the physical system consists of the pollutant-laden atmosphere. The initial state must be determined by appropriate measurements. The time-variable influences are, on one hand, of a purely meteorological type, such as solar radiation, precipitation, etc., and on the other hand, the sources of harmful materials near the ground. From the knowledge of initial conditions and external influences we are generally able to compute in advance all future states of the pollutant-laden atmosphere. This problem is solved by "mathematical-meteorological diffusion models" which thus make up the most important element in any air quality maintenance control strategy.

1. MATHEMATICAL-METEOROLOGICAL SIMULATION OF AIR POLLUTION SITUATIONS, IN GENERAL

It has been emphasized that every control strategy requires the most reliable possible immission prediction. This prediction can extend in time from perhaps one hour up to years and decades, and can cover spatial regions of individual points up to a significant part of the earth's surface. The quality of such predictions depends decisively on the quality of knowledge and predictions of the emission register, and also on the quality of the predictions of atmospheric states. At present, the quality of predictions of the temporal changes of the emission register as the result of variations with the time of day or as the result of long-term industrialization is just as unsatisfactory as that of the predictions of the atmospheric states. This situation, then, currently prevents the rational development of control strategies, which are pressingly needed. In spite of this, we must do what we can at present with the existing scientific aids in order to help avoid the grossest planning errors in the field of air quality maintenance.

1.1 On the concept of mathematical-meteorological simulation

In nature, the pollutants which enter the atmosphere are transported away from the sources in an extremely complex manner and "diluted" by the effect of atmospheric turbulence. In a later chapter, we attempt to make the problems which occur here understandable. Due to the great variability of all atmospheric properties, there is no hope at all of giving a complete description at every time of this "transmission" process, which in the causal chain

EMISSION – TRANSMISSION – IMMISSION

makes up the connecting element between the sources of the harmful material and the receptors. There is only the possibility of approximating this transmission mechanism sufficiently accurately by means of a suitable mathematical-physical-meteorological model. Such approximate modeling of a physical process is called "simulation". If we are successful in understanding the most important parameters sufficiently well in the model for a given problem, then we have a simulation which is adequate for the problem. The problems posed in the field of air quality maintenance determine from the beginning the character of the modeling of the transmission process. Then it depends on the knowledge of the modeler whether or not the simulation of transmission satisfies the requirements of the practical problem. Typical problems in the past were: How does one determine the minimum design height of industrial smokestacks which are to be newly built, from the viewpoint of minimum pollutant stress on the near and far environment? How, in industrial and populated areas of congestion, does one determine the basic immission stress already present and to be expected later? How does one solve the problem of location selection for industries to be established anew, or the problem of planning new housing areas in populated regions? In such populated regions, how does one arrive at a prediction of the occurrence of particularly high emissions and, thus, at the development of a warning system for the population and a control system for the emitters? All these questions and many others which occur to us can be answered only with the help of simulation of the corresponding transmission conditions.

The method of model simulation is relatively new in the field of air pollution control and has not yet permeated it entirely, although it has been obvious to physicists and technologists since the beginning of modern science. From the field of meteorology, let us only mention the model simulation of the changes in state of the atmosphere which has led to very useful theoretical weather predictions. But we must always keep in mind that such a model simulation represents only a more or less good approximation of natural conditions, and that "perfect" results can never be obtained; but, they are also not required in many practical problems.

1.2 Emission, transmission, immission and planning as parts of a control system

Any air pollution control strategy must make use of control theory, which has become highly developed in our time. Expressed generally, this is a matter of the following: Let a reactive system (such as the atmosphere) be given. We introduce a certain "input" to this system (e. g., air pollutants). The system processes the input and produces an "output" (e. g., harmful effects on the vegetation) which is evaluated. If the output does not agree with the requirements (maintainence of limiting values) then one doubles back to the input through the control section, changes it, and observes the effect of this measure again at the output side. We reiterate this control loop until the output agrees as accurately as possible with the requirements. If this system deals with prediction, then we have carried out a control strategy. We shall demonstrate this manner of thought with the example of a typical problem in the field of air quality control.

Our system consists of the atmosphere and the earth's surface. The entire transmission process is determined by what the atmosphere does with the introduced pollutants in interaction with the earth's surface. As the input for the system we have, primarily, the local emission register of the closely observed region. But, in addition, air already polluted can be transported by the atmospheric flow system from more distant population centers to the area under consideration so that the immissions of the distant sources and those

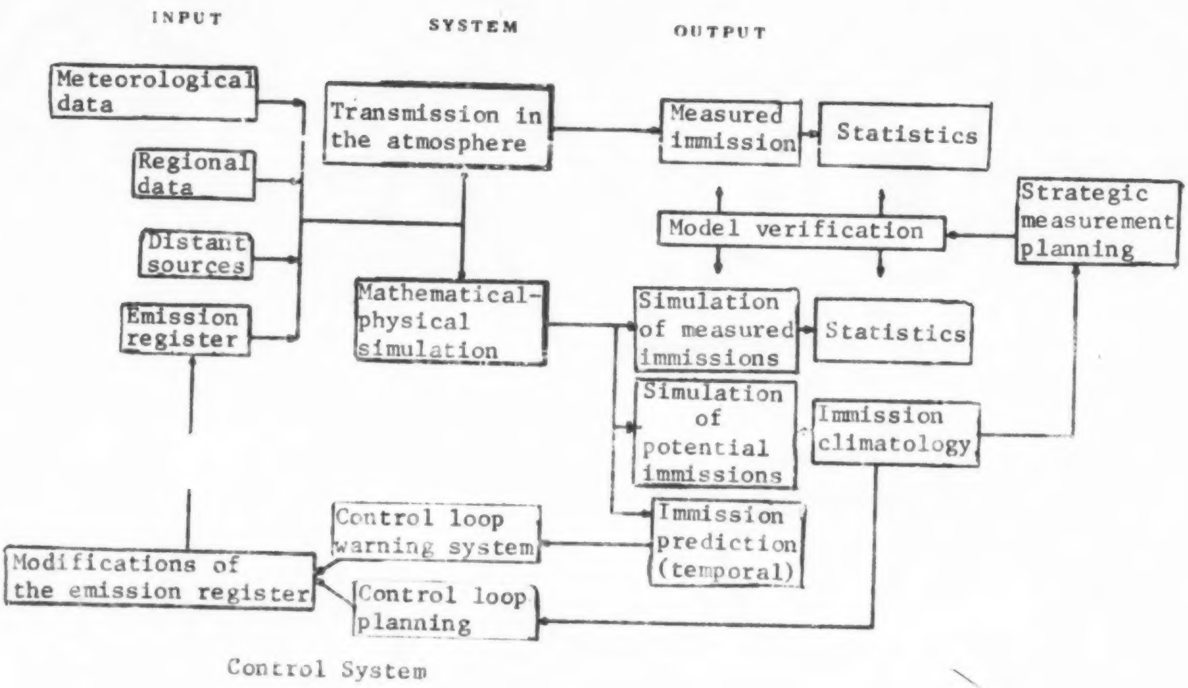

INPUT
SYSTEM
OUTPUT
Meteorological data
Regional data
Distant sources
Emission register
Transmission in the atmosphere
Mathematical-physical simulation
Measured immission
Statistics
Model verification
Strategic measurement planning
Simulation of measured immissions
Statistics
Simulation of potential immissions
Immission climatology
Immission prediction (temporal)
Control loop warning system
Control loop planning
Modifications of the emission register
Control System

Figure 1. Control loop in the field of air quality control.

of the region are superimposed. Their rather even spatial distribution is characteristic for the immissions of distant sources, due to the basic mixing along the long transport route, among other things. Along with these input data on emissions there are primarily the meteorological data which cause transport and mixing of the air admixtures. For a certain point in time, these are the spatial distribution of wind strength and direction, the horizontal and vertical temperature conditions, and the radiation, cloud, and precipitation conditions. From the given meteorological parameters, with the not inconsiderable influence of the character of the earth's surface, there follows the spatial distribution and the intensity of the atmospheric turbulence. This leads to the very effective process of "dilution", by making possible the turbulent diffusion of air admixtures. As an input parameter, the nature of the earth's surface has a part not only in the development of atmospheric turbulence, but also in the development of the low-level wind systems, if we are dealing with hilly terrain, and due to the fact that adsorption of pollutants is possible at the surface. We need quite accurate information on these four groups of input parameters shown in Figure 1, under all circumstances, whether we wish to make reasonable interpretations of measured immissions, or whether we are thinking of a model simulation of the immissions due to the input. Different requirements for the extent and accuracy of the input parameters are set up, depending on the problem.

In nature, the data input unambiguously defines the output. This consists of the immissions which occur at the earth's surface, and which are subjected to very strong temporal and spatial variations. This follows solely from the great variability of the meteorological input parameters; but, the irregular spatial distribution of the emissions also leads to corresponding spatial variations of the immissions. Covering large errors presents considerable difficulties for measuring technology. It is entirely conceivable that for purposes of city planning in the future someone will need the time course of the immission values (perhaps half-hour averages) at points within the area of concern, separated by no more than 500 meters. This is necessary, among other things, in carrying out a correct control strategy; but also if an immission climatology is required with an accuracy optimally describing the conditions of European cities. It is apparent that a measuring network with such high temporal and spatial resolution is not within the range of possibility. A stronger argument against the construction of such costly measuring networks is the fact that no prediction is possible on the basis of measured immissions which at times and under certain circumstances can be derived from far distant emissions, because they are exclusively past-oriented, and therefore suited only for the description of what was once the case, on the basis of emission conditions and meteorological diffusion conditions.

The situation is quite different if it is possible to simulate the transmission process with a model. In the most general case, we deal with a physical-meteorological model, formulated in the language of mathematics, which must be able to compute the time course of the immission with arbitrarily high resolution and for arbitrarily many points within the region considered, for the same period for which the input parameters were predicted, on the basis of predicted meteorological parameters and predicted course of the emission condition. This type of immission prediction is closely linked with theoretical weather prediction; but in the ideal case this yields the prediction of the meteorological parameters relevant to transmission. Methodically, too, both predictions are quite identical.

The exact prediction of the time course of immissions in a congested area is a wish like that for accurate weather prediction. There are many basic reasons which oppose accurate prediction of the meteorologic parameters responsible for transmission. We shall discuss them later; but, if we had a "sufficiently accurate" prediction (where the definition of the concept of "sufficiently" can be established only on the basis of the problem), then we could develop a true control system to maintain immission limits in a congested area for all of the merely possible meteorologic situations. From what we said previously, then, this would appear as follows: The mathematical-meteorological diffusion model, which provides a model simulation of the time course of the immissions, reacts as a system to the time-variable input of emission data and meteorological data, which were predicted separately, giving the time-variable output , the immission field of the region. All this occurs within an electronic computer. The computed and stored immission fields are then tested internally by a program which determines whether the immission limits are exceeded at some time and/or at some point. If this is the case, then a fixed control strategy program goes into action as follows: Depending on the weather situation (and primarily on the wind direction), the emissions of the input are partially reduced in a first approximation. With the emission input thus reduced, the immission prediction is undertaken again, tested internally for excesses over the immission limit and, if there are still excesses, the experimentation is continued by renewed modification of the emission conditions until it is ensured that the immission limits are not exceeded anywhere and at anytime during the prediction period. This internal computer process to perform a control strategy can be programmed so that it runs quite automatically in a short time and also considers economic viewpoints, to the extent that cost problems can play an important role in choosing those emitters which must reduce their emissions. That is, if we can reduce the exceeding of the immission limits by reducing emissions from "cheap" emitter groups, this would be a quite important aspect of a reasonable control strategy. In the ideal case, one could warn all operators of air-polluting emitters with sufficient accuracy for one to three days,when and how much they would have to reduce their emissions.

This control system, once developed for one region, would be so flexible that it would require only minor cost to consider the increase in the number of emitters in the emission register which occurs with further industrialization and opening up of the region. Inside the computer, the operation of the control loop would not be changed in its programming by the increase in number of sources. Until today, no such automated control system has existed, although it is within scientific possibility. One reason for this situation is the minor interest, until now, in doing research on the development of emission-oriented simulation models for the transmission of foreign substances in the atmosphere, so that no research center training a new generation in this field could have developed. It will be apparent to anyone who considers the principal difficulties in this undertaking that a considerable amount of basic research is yet to be done for realization of this goal. An unconditional prerequisite is the existence of a complete emission register of all emitters and all the foreign substances given off into the atmosphere. Without an emission register there is no rational control strategy and no reasonable immission-oriented city and regional planning, as we shall see later. Here, many problems are yet unsolved: How must the emission register appear with respect to temporal and spatial resolution to carry out the previously described control strategy? How great must the accuracy be for the present purpose? What accuracy is worth while in view of the possible inaccuracy in the determination of the other parameters, and particularly of the meteorological parameters? These and other questions about the emission register can only be answered after development of the simulation model, because the model, considered as a picture of our atmosphere-ground physical system, reacts very differently to the different input parameters. The sensitivity of the model to inaccuracies in the input parameters would appear in the assigned inaccuracies of the computed immission fields. These inaccuracies can certainly be evaluated to some extent by comparison with measured immissions. If one installs suitable recording measuring instruments at a certain number of "representative" points within the region, then one can simultaneously compute the immissions found there according to the model from the emission register and from the meteorological situation. Then one has not only the possibility of verifying the model, but also of investigating the model with respect to its sensitivity to errors in the model assumptions or in the input parameters. It can then be found as a result that large sums can be saved in collecting the emissions due to lower accuracy requirements for the emission register. Another unconditional prerequisite for attaining the goal is intensive basic meteorological research in the direction of the temporal prediction of those parameters which are of decisive importance for the transmission process. The facts that we are dealing with predictions for areas considerably smaller than the so-called synoptic net of the weather service, and that the hourly course of the meteorological parameters can be significant here, allows quite little of the information now being provided by the weather service to be applied for this purpose.

The latter fact becomes particularly clear if we consider how strongly the transmission must depend on the local topography of the country. Of course, the conventional predictions of the meteorological parameters cannot go into this influence. In summary, one can in any case establish now that no air pollution control system of the desired type can be developed because of the difficulties mentioned.

The short-period immission prediction, as a prediction of the time course of the immissions, represents an important problem, but not the only one, in the field of air quality control. Long-term immission predictions have by far the most importance for future planning of our environment with respect to air cleanliness. This subject is called, in German, "Immission-Grundbelastung" ["Basic Immission Load"]. So far, it has not been possible to translate this concept into English, or to explain it convincingly to English-speaking colleagues. Even in the German language, there is no unanimous clarity on the meaning of this concept, although TI Air [1] gives some guidance as to its measurement (see also [2]). The author of this study has used immission frequencies to define the basic immission load [3, 4, 5] and will refer back to this definition in the discussion of the model.

If we record half-hour averages, for example, of the immission over a long period of time at many measuring points within a congested area, then one can produce an immission map of the region from all the measurements for each half-hour interval. Due to the variability of the meteorological parameters and perhaps also of the emission conditions, successive maps will generally not agree. If, for instance, one makes such immission maps for an entire heating period, then, from about 200 heating days one would obtain 48 x 200 = 9,600 such maps of half-hour immission fields. Now, if we film these maps and project the film at a rate of 16 frames per second, then we would experience the time course of the immission in the whole region in 10 minutes. This would appear as follows: each immission map contains a system of lines of the same immission (e. g., for sulfur dioxide, isolines for immission steps of 0.1 mg/m^3). These line systems would move as the film was projected. New centers with higher immissions would appear and vanish again. The major points of immission would shift, depending on measure of the weather situation in the congested area, among other things. Purely visually, through a sort of internal brain statistics, one would have found what areas of the total congested region one would choose for himself as a place to live, and which he would never choose. But with this sort of visual statistics, one would have produced within himself an accurate picture of the basic immission load of the whole region during the heating period of concern.

The process can be shaped somewhat more objectively with the aid of simple frequency statistics. One sorts the 9,600 half-hourly averages at all measuring stations into a limited number of immission classes and counts how many immission values occur in each of these classes. This gives a frequency distribution of the immission values for each of the measuring points. One would not be able to distinguish all of these, from potentially thousands of measuring points required. The statistical properties of frequency distributions, such as the mean, most frequent value, and many others, however, can be calculated very easily from the frequency distributions determined. One could have established these statistical properties only visually in watching the film. Only these are usable for evaluating the basic immission load. It is a characteristic of the frequency distributions of immissions that they undergo relatively strong spatial changes within the congested region. This is related, on one hand, to the irregular arrangement of the sources; and on the other hand, the frequency statistics provide the meteorological parameters for these spatial differences. For this reason, the statistical characteristics of the frequency distributions must change from measuring point to measuring point, and one is able to draw maps of the statistical characteristics of the immission frequency distributions, analogous to the individual immission maps. Then these alone represent the basis for definition of the concept of the basic immission load.

If one performs this process for successive heating periods, then one establishes that the previously drawn map of the basic immission load changes from year to year. One reason for this is that the course of the meteorologic conditions can be quite different during the heating periods. Also, the emission conditions change systematically in the sense of an increase in emissions. The immission basic load is primarily a function of the time, depending on the proportion of the time dependence of the emission conditions. The dependence on the meteorologic conditions which vary from year to year must be eliminated, however, because for the purpose of future planning at least one complex parameter must remain constant. Here, climatology appears useful for application to the transmission conditions of the region of interest. By observing the transmission conditions in the atmosphere for many years it is possible to determine a standard course of the meteorological conditions during each period of the year, such as the heating period, and to use this as the meteorological input for the model computations. As one is using climatologic transmission parameters, one calls the output of the model computations, i. e., the immission frequency distributions for each point of the region, immission climatology. The first model for computation of an immission climatology for a city has been developed by the author for the city of Bremen since 1962. The first emission register for sulfur dioxide also originated there in 1964.

Now let us return to Figure 1. We cannot expect production of data for construction of half-hour immission maps from measuring technology. Even if we did not dread the high financial costs, we would have the problem mentioned above, that the conditions change from year to year for meteorological reasons. Future projections in the sense of rational city planning are also impossible; but, the situation is different for model simulation of the immission climatology. If one has a model which is able to calculate a sufficiently accurate immission field from knowledge of the weather conditions for any weather condition occurring, then the previously mentioned film of the course of the immission conditions during a certain period of time can be produced quite easily with the help of immission maps computed by the computer and drawn with an electronic drafting device. This would then be a standard course, as climatological values are used for the course of the transmission conditions. As the immission frequency distributions are also calculated and stored in the computer, their statistical characteristics can be computed easily and drawn automatically in the form of maps.

This would open the way for the solution of many problems in the field of air quality maintenance. In particular, let us now close the extremely important control loop of city and regional planning in the following sense. On the basis of a current emission register and the transmission climatology of the region, we calculate the immission climatology for different time periods of the year, as for the months separately, for the seasons, or for the heating period and the heatless period. Here one may find that the basic immission load, derivable from the immission climatology, in certain areas of the congested region already exceeds certain limits which, to be sure, are yet to be established by the legislature. Here, then, supplementary aids must be provided, either by moving industrial districts or by special technical measures to limit emissions. But the model shows its true value only in the planning of new industrial and housing areas. If new groups of emitters are planned in the region, then one can add their planned emission data to the emission register and, with the model, predict the immission climatology as it would occur after installation of the new plants. If we establish in that way that the limiting values for the basic load are exceeded in certain areas after installation of the new plants, we carry out variations of the data for the planned plants within the computer so that after multiple iterations of the control loop, there are no longer any exceeding of the limits. These variations of the plant parameters (including the intended location) can obviously be performed with consideration of optimal economic boundary conditions for all participants. At present, the problem of immission-oriented city and regional planning is the most pressing one in the field of air quality maintenance. By omissions and erroneous planning in this field, we not only have a negative effect on our own future position, but we cause irreparable damage for the following generation. Fortunately, we have, for some years, had available the scientific fundamentals for such planning problems, with which these problems are even today being solved.

This optimistic position is based on the author's long work on the problem. In view of the extraordinary complexity of the problem, it contradicts a considerable pessimism of colleagues who have not themselves been concerned with model developments. In fact, the problem of model simulation of air pollution situations appears so hopelessly complicated, from the viewpoint of those who are concerned with all possible influences on the transmission process, that all belief in theoretical solutions can be lost in the sense of model simulations. In the next chapter, we shall pay particular attention to these difficulties and show what research still has to produce in order to arrive at reliable statements for prescribed problems in the field of air quality maintenance.

2. PHYSICAL, PHYSICAL-CHEMICAL, METEOROLOGICAL AND MATHEMATICAL PROBLEMS OF MODEL SIMULATION

In the model simulation of the transmission process, not only are meteorology and physics called into the plan, but along with mathematics, recently also in particular, physical chemistry and air chemistry. Thus, if we consider the many branches of technology working together on the side of emission, and those of medicine, botany, and legislation on the side of immission, then our problem proves to be very much an interdisciplinary one. Following a presentation by W. Breuer [2], we shall in the following first discuss, rather in one lump, the various quantities influencing the transmission process. In the upper part of Figure 2, the meteorologic input of Figure 1 is shown in expanded form. The emission register, as an input, appears in the center as emission, and the regional data for the input side appear at lower left. The process of washing out the photochemical reactions and the chemical reactions during the transport of the air additives in the atmosphere have not been mentioned before.

As atmospheric air is the transport medium for the air pollutants, the meteorologic parameters are ascribed the principal importance in the occurrence of transmission. On rather superficial consideration, there are only two parameters at first which determine the transmission: the horizontal wind field, averaged in some manner, and the degree of turbulence of the flowing air. If the wind field alone were responsible for the transmission, it would be possible to develop transport models for pollutants very easily because the amount added to an air quantum would remain in this quantum and one could move it along the path of the air quantum (trajectory). Then the only remaining problem would be determination of the trajectory of the air. Unfortunately, atmospheric turbulence works against this simple scheme. The small-scale disordered motion of the air, which is superimposed on the average motion (measured wind) causes the foreign substance in the air to diffuse to all sides out of the air quantum which is being moved along the trajectory. This produces very considerable differences in the transmission process in comparison to the simple displacement method.

The average wind field in a large industrial complex is in many cases determined by the large-scale weather situation and, so, to a good approximation, by the large-scale air pressure distribution. The wind direction plays more the part of a selection parameter, as it selects those regions which can be stressed by the emissions from the source region.

But, with an inhomogeneous soil stratum, it can occur that the mechanical turbulence generated from ground unevenness and from roughness depends on the direction of the incident flow. The

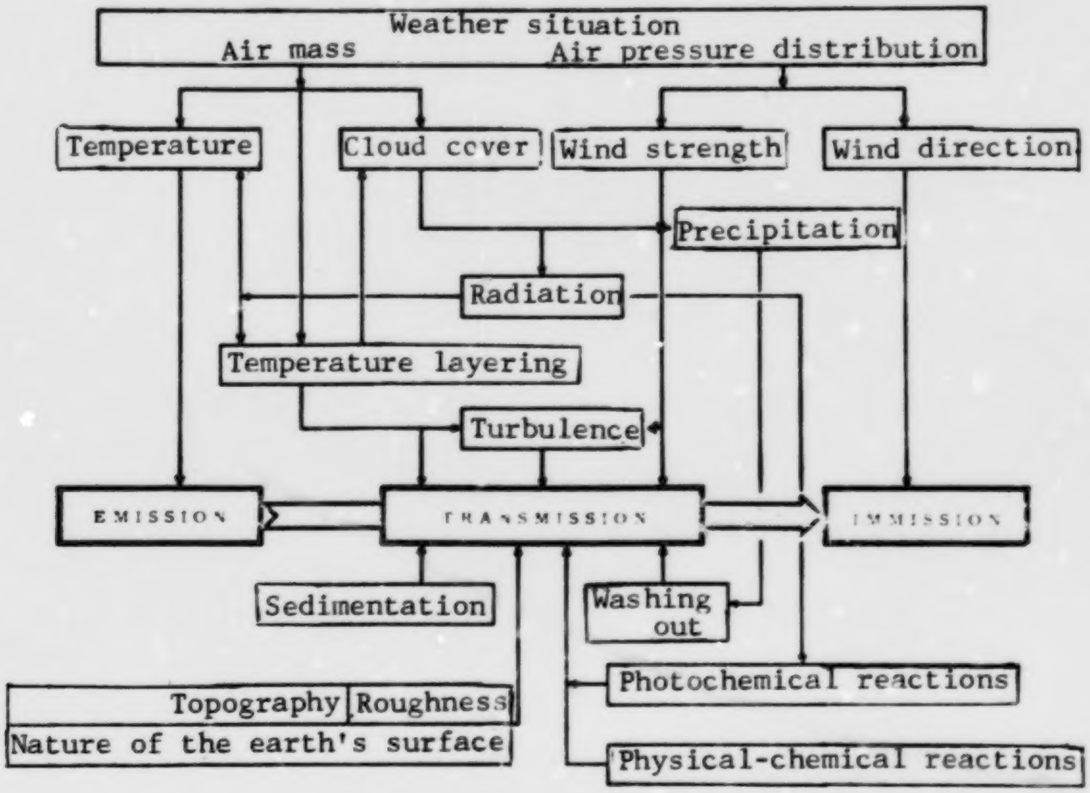

Weather situation
Air mass
Air pressure distribution
Temperature
Cloud cover
Wind strength
Wind direction
Precipitation
Radiation
Temperature layering
Turbulence
EMISSION
TRANSMISSION
IMMISSION
Sedimentation
Washing out
Photochemical reactions
Topography
Roughness
Nature of the earth's surface
Physical-chemical reactions

Figure 2. Parameters influencing transmission.

wind strength, along with its effect on the transport process, also has great importance for the development of the intensity of the turbulence. The degree of air turbulence is also determined by the particular properties of the air mass in which the congested area is. The existing cloud cover has a decisive effect on the radiation conditions. These affect the temperature distribution, particularly the vertical temperature layering, on which the development of atmospheric turbulence depends very decisively. The development of clouds is also very dependent on the vertical temperature layering, which yields a loop of the dependences of the meteorological parameters. This complex interaction between the different meteorological parameters is what makes it so extraordinarily difficult to predict the turbulent state of the atmosphere. It has already been mentioned that the nature of the earth's surface participates significantly in the development of the character of the turbulence. In many cases, also, the ground topography causes modifications of the large-scale wind field near the ground. These can develop into local circulations which apparently have nothing more to do with the large-scale wind field (although, of course, they are generated by it). In this respect, we can consider the wind distribution in valleys, which is extremely affected by the topography.

Small-scale wind field structure and atmospheric turbulence determine the transport and the turbulent diffusion of all additives to the air decisively, and lead to an immission which can be related unambiguously to the emission, if the air pollutants were exposed to nothing more than the transport processes in their path through the air. This simple situation usually does not occur. Sedimentation of dust in the gravity field and washing out of gases by precipitation are two processes which, like settling, act on the air additives during their transport, preventing the unambiguous relation of emission and immission through the meteorological transport and diffusion process. This is limited even more seriously if foreign gases in the air enter into chemical interactions with each other or with the permanent components of the air during transport. In this way, space-time-dependent decreases for the emitted gases occur in the atmosphere. At the same time, new gas components are formed through the chemical interaction in the atmosphere.

2.1 Physical problems in simulation of transmission

Even though meteorology, as the physics of the atmosphere, is more and more coming to the attention of the other natural scientific disciplines, there is still a whole series of problems of model simulation of air pollution situations outside of meteorology. These problems can be solved only with the help of the methods of theoretical physics. These include, particularly, a physically well-based theory of turbulence and of turbulent diffusion. Great advances have been made both theoretically and experimentally in the field of wind tunnel turbulence. In comparison, little is known theoretically about the origin and development of atmospheric turbulence. One reason for this situation is the unusually great spectral range of phenomena which one must include in atmospheric turbulence. Another is related to the fact that atmospheric turbulence depends on a great many parameters. These are included, on one side, in the large-scale (synoptic) meteorology and, on the other side, in the character of the earth's surface. The result is that a mathematical equation for the turbulent diffusion of air additives is always coupled with the mathematical equations for description of the large-scale meteorological parameters. Perhaps an example will explain this better. In the emission and transmission of dust, the radiation conditions in the area of dispersal are changed, not insignificantly. This influences the temperature distribution within the atmosphere, the development of certain types of cloud cover and finally, then, the development and the character of atmospheric turbulence. The change in the turbulence has its effect in a change of the spread of the dust, and the whole action begins again through feedback. It is very difficult here to predict theoretically what state will appear as the steady state at the end, and how long it will last, until it is reached. Such feedback and interaction mechanisms are characteristic of the atmosphere. They impede every type of prediction, including those in the area of air quality maintenance. Here, too, is one of the principal problems of physical turbulence research. Other problems are of the pure flow physics type. As yet, there are hardly any models for flow around and over ground elevations, for the circulation systems in valleys and basins, and not even in a satisfactory way for the flow conditions induced by skyscrapers in population centers. In all cases, we can proceed from the fact that a large-scale flow, little affected by the nature of the topography, is present at a height of 1,000 to 1,500 meters above the ground. The modification of this flow within the planetary boundary layer, as the layer below 1,500 meters is named in meteorology, is a problem which is essentially unsolved; but, it is this layer in which the transport and turbulent diffusion of air additives primarily occurs. The situation is simple only in the case of congested regions which are located in completely flat terrain and which have a low proportion of skyscrapers.

Other physical problems are concerned with the height to which hot smoke plumes rise before they are also diverted horizontally by the horizontal wind flow and then become subject to turbulent diffusion. Here we are dealing with a hot free jet which is ejected vertically, perpendicular to the horizontal flow, from a small source (smokestack opening) at a certain velocity. Initial velocity, thermal lift in the air in the vicinity of the opening, which is generally colder, interaction of the jet turbulence with the turbulence of the air, and vertical temperature stratification determine the so-called effective stack height, made up of the stack construction height and the stack overheight, in a very complex way. As the maximum ground immission generated from a smokestack depends very sensitively on the amount of stack superelevation, a theory for the free jet is of central importance for the answering of problems of air quality maintenance; but, no such theory yet exists.

2.2 Meteorological problems and their current pragmatic solutions

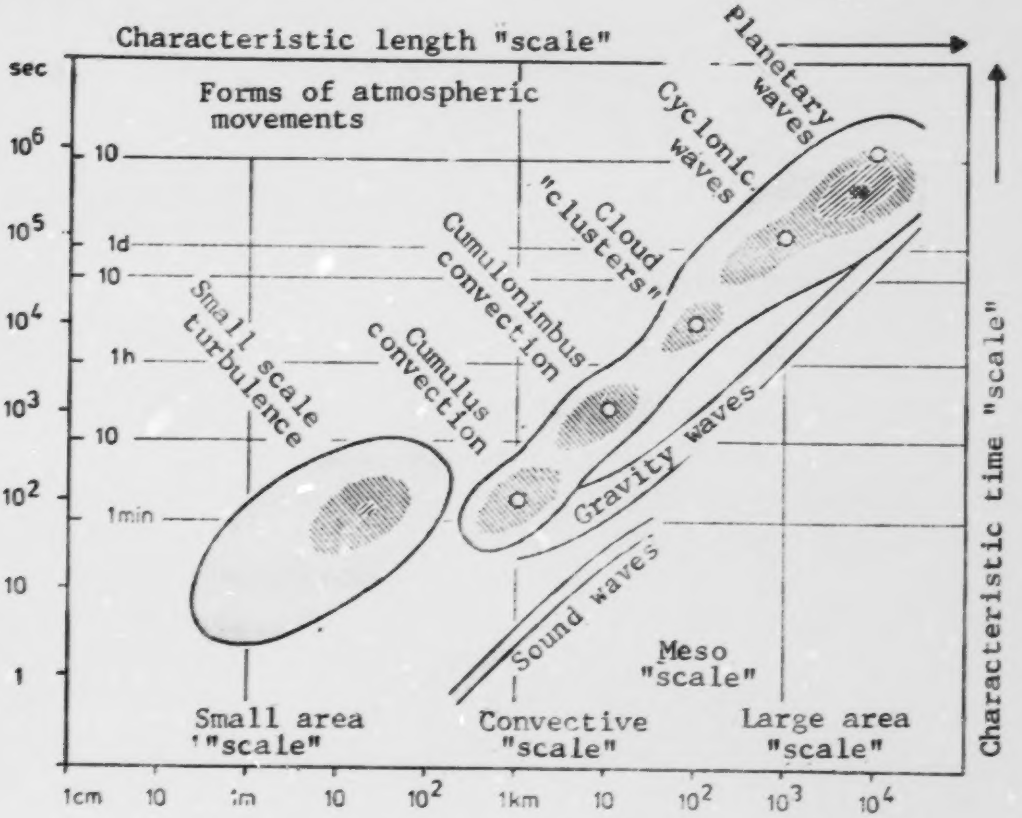

Characteristic length "scale"
Forms of atmospheric movements
sec
10^6
10^5
10^4
10^3
10^2
10
1
10
1d
10
1h
10
1min
Planetary waves
Cyclonic waves
Cloud "clusters"
Cumulonimbus convection
Cumulus convection
Small scale turbulence
Gravity waves
Sound waves
Meso "scale"
Small area "scale"
Convective "scale"
Large area "scale"
Characteristic time "scale"
1cm
10
1m
10
10^2
1km
10
10^2
10^3
10^4

Figure 3. Orders of magnitude of forms of atmospheric motion.

One typical meteorological problem, which plays a large part in the area of air pollution, is related to the fact that there are motion phenomena and processes in the atmosphere which extend over enormous orders of magnitude with respect to spatial extent and temporal duration. This fact may be explained briefly by means of Figure 3 [6]. On the basis of observations of quite different types, we can divide all phenomena roughly into four size classes. The first class contains all the phenomena of small-scale turbulence, which we have already spoken of, which occur primarily within the planetary boundary layer; that is, in the lowest layer up to a height of 1,500 meters. For these small scale air turbulence phenomena of limited life, we can represent the spatial size by a characteristic length "scale" and the lifetime by a characteristic time "scale". Turbulence eddies which occur rather often have "diameters" of about 10 meters and lifetimes of about 1 minute. This type of eddy can often be observed well in smoke plumes. The size and lifetime of the eddy, considered generally, the spectral distribution of the eddies, and their lifetime decisively determine the process of turbulent diffusion within the planetary boundary layer. The action of small-scale turbulence is ascribed the greatest significance in all model simulations of air pollution situations. But under so-called unstable conditions (see later) conditions occur in which the turbulence eddies reach sizes such as are found for transition to thermal convection (100 meters or more). These large eddies with lifetimes of perhaps 10 minutes lead to a very intensive turbulent mixing and, therefore, to strong turbulent diffusion in the vertical direction. Here brief peak values of concentrations occur at the ground, but in all, there is rapid transport of the air pollutants away from the ground to higher altitudes.

On days of intensive irradiation, the air layers strongly heated near the earth break loose in the form of thermal bubbles at more or less regular intervals. Due to their thermal lift, these rise by themselves. This thermal rise is superimposed on the already-present turbulence of the air. At high altitude, but still within the planetary boundary layer, several such thermal bubbles flow together and cause the development of cumulus clouds above 1,000 to 1,500 meters. Proper attention has not yet been given to the significance of this process in the spread and transport of air pollutants. As the thermal bubbles flow together, the foreign materials in the air are to a certain extent drained together, carried upward in narrowly limited vertical channels, and redistributed at heights above 1,000 to 2,000 meters. Restored downward transport into the lower layers is greatly impeded by the facts that in the region between the thermal tubes, only a very slightly sinking air motion is found, and that turbulent diffusion is relatively slight at these heights. This vertical, organized transport of air pollutants away into high layers of the atmosphere occurs even more effectively in the large and very large source cloud regions, which occur particularly often in the summer, but also with penetrations of cold air during the other seasons. It is still impossible to predict the occurrence of thermal convection, the number, size and life of cumulus clouds, or the effects which these systems produce on the transmission process. Often vigorous thermal convection is found in high pressure weather conditions in which the large-scale horizontal wind system is very weakly developed; but, for turbulent diffusion under low wind conditions, we still lack simulation models and, especially, measurements of the relevant diffusion parameters.

The region designated as meso-"scale" in the diagram of Figure 3 includes phenomena of the magnitude of about 100 km and lifteimes of about 10 hours. These include, for instance, the circulation in the region of a local heat island which develops over congested regions in the summer. Then we have not only the effects of small-scale turbulence along with those of thermal convection, but a superimposed flow directed concentrically into the interior of the city. This leads to a strong accumulation of air pollutants which are more or less effectively carried away to high altitude by vertical movements of the air. For this type of air pollution situation, too, there is still no model simulation.

The fourth large group of phenomena in the atmosphere is formed by the large vortex systems generally known under the names of cyclones (low pressure vortex) and anticyclones (high pressure vortex). While some problems of turbulent diffusion in high pressure weather conditions were described previously and turned out to be relatively difficult due to the occurrence of thermal convection, the situation is much simpler, in comparison, in low pressure weather conditions. Here we usually deal with strongly developed flow systems which lead, through transport and diffusion of air additives, to a more easily described "dilution". But here again there remain a large number of unsolved problems. Something has already been said about the effect of inhomogeneous horizontal wind fields on the transmission process. The occurrence of this inhomogeneity is conditioned not only by the topography, but also as a result of the large-scale wind fields if the prediction area for which an air hygiene model was developed is large enough. Convergences of the wind fields lead to accumulations of air pollutants in the convergence regions. Divergences cause additional "dilutions" which are superimposed on those from turbulent diffusion. So far, there is still no simulation model for congested areas which is able to take into consideration the effect of nonhomogeneous horizontal wind fields. Another important effect related to the horizontal wind field structure has not yet been worked out: If air flows from a region of great ground roughness to an area with less roughness, or conversely, then there occurs a modification of the horizontal and vertical wind structure as well as a corresponding change of the turbulence conditions. Changes in the wind direction after adaptation to the new surface are not uncommon with appropriate jumps in roughness. Also, vertical movements are often generated in the adaptation process, and these affect the transport of air additives.

The vertical wind structure is also of great influence on the transmission process. The vertical wind and turbulence structure within the planetary boundary layer is one of the most currently important research objects of modern meteorology, not least because it is so closely linked to the solution of air pollution problems. Depending on the vertical temperature stratification, we find a strong layer below 20 to 100 meters in which the wind velocity increases with height from zero at the ground without changing the direction of the wind. Furthermore, a further increase in the wind velocity occurs with changes in the wind direction until, at the upper boundary of the planetary boundary layer, the strength and direction of the wind agree with those of the large-scale wind vector of the free atmosphere. The turbulence increases, from a value of zero in the immediate neighborhood of the ground, assumes a maximum value in the middle of the planetary boundary layer, and decreases again to zero at its upper limit. This wind and turbulence distribution in the vertical affects the transmission process quite considerably. The fate of a smoke plume, and, as a result, the ground immission, depends very much on the height of emission above the ground. For emission heights below 100 meters, the problem is not yet very critical. Due to the wind direction being constant with height, horizontal deformations of the smoke plume do not occur as they do in the case of a wind direction varying with height. Also, in many cases the wind velocity can be replaced by an average one applying to the whole propagation layer. We need not go into the technical details in this relation here. The whole literature of the spread of smoke plumes treats this problem. The spread of waste gases in the case of height dependence of the wind direction and of the spread parameters is not treated. Large emitters have construction heights of more than 200 meters. The thermal lift of the hot smoke gases leads to stack superelevations of the order of the construction height. The effective stack height is then about 500 meters; but, at this height the wind direction is distinctly different from that near the ground, usually in the sense of a deflection toward the right. This has the result that lines of equal concentration in cross sections perpendicular to the wind direction have a distinct tilt from the lower left to the upper right, if we look in the direction of the wind. LIDAR measurements on smoke plumes have clearly confirmed this effect. It is apparent that different ground immissions will be generated under these conditions than in the case of a constant mean wind vector for the whole layer. Trial solutions for modeling the propagation in such a wind field varying with the height already exist and could soon be built into the model for the most varied problems of air quality maintenance. Thus, the model would presumably be used for a considerable improvement in determination of minimum smokestack heights. Unfortunately, meteorological data about the wind deflection within the planetary boundary layer are still too sparse. Routine measurement of the vertical wind structure within a region of the size of a population center is ruled out because of the costs. There remains only the possibility of making a conclusion about the wind structure indirectly from existing simple measurements at the meteorologic stations. This is called the parameterization of a small-scale phenomenon using parameters taken from the large scale. That is, these parameters are routinely measured at large time and space distances. This problem, too, is now a central point in meteorologic research and is still far from solution.

The conditions are quite similar in determining the ability of the atmosphere to "dilute" additives introduced through turbulent diffusion. As previously established, theoretical physics has not yet produced any theoretical aid which would make possible the determination of the diffusion parameters. In connection with Figure 2, we attempted to make understandable the influences which affect the atmospheric turbulence. Along with the wind strength, the vertical temperature stratification of the atmosphere appeared to be a significant influencing parameter. In meteorology, one can show that a vertical temperature decrease of some 1°C per 100 meters occurs very often within the planetary boundary layer, and that a so-called indifferent (neutral) layering is related to this value. With this layering, vertically displaced air quanta are always in thermal equilibrium with their new surroundings, simply because the adiabatic temperature change of the moved air quantum also has the value of 1°C per 100 meters. When the temperature decreases more strongly with the height, e. g., 2°C per 100 meters, an air quantum cooled adiabatically by 1° after 100 meters of rise would no longer be in equilibrium with its surroundings because of its overtemperature. It would experience thermal lift and would rise farther by itself, with acceleration, because the temperature difference from the surroundings would steadily increase. Such a vertical temperature layering is called unstable. Any small disturbance of the air quanta from a rest position leads immediately to rearrangement of the whole air mass, which produces a particularily strong turbulence. Conditions are opposite in the case when the vertical temperature distribution is less than in the neutral case, 0.5°C per 100 meters. An adiabatically rising air quantum cools off by 1°C per 100 meters, and arrives cooler than the surroundings there. As a result it suffers a downward force and finally oscillates about the resultant position (until friction brings it all to rest again). This layering is called stable. It is also not to be expected that strong turbulence can arise in such a situation. Every type of vertical motion is more or less damped, depending on the vertical temperature gradients. The occurrence and the intensity of the turbulence are, then, closely linked with the stability of the vertical layering. Thus, this stability has also been used as a measure for the turbulence itself. The extreme case of unstable layering (more than 2 to 3°C per 100 meters), where extremely strong turbulence is possible, contrasts with the extreme case of stable layering, in which the temperature actually increases with the height. Within such a stable layer with temperature inversion (thus the name, inversion layer) the origin of turbulence is practically ruled out, and turbulent diffusion as well, so that an inversion layer acts like a solid barrier layer for the turbulent transport of air additives.

There are studies which indicate that the magnitude of the wind velocity and the vertical stability of the temperature layering are sufficient parameters to characterize the intensity of the turbulence. Then one would also have an appropriate characterization for the turbulent diffusion. Unfortunately, the conventional routine observations are not adequate in this field, either. In particular, systematic vertical temperature probes are lacking. These must be done at many locations within the congested area, regularly and with high resolution, particularly in order to pick up the low inversions. Inversion, as a barrier layer of decisive importance for upward exchange, is the primary determinant of the course of temporal growth of low-level immissions in many critical air pollution situations. Attempts at routine monitoring of the vertical temperature distribution are still very sparse, and they are usually also quite expensive financially. The usual radiosonde ascents are not suited for such purposes because at best they determine the temperature distribution above 200 meters, and that quite inaccurately. Fixed balloon ascensions with fine meteorological sondes are much better suited, but they cannot be carried out everywhere because of flight safety reasons. New possibilities are provided through the development of acoustic radar. This is an instrument which is not cheap, certainly. The cheapest and most reliable method for determining the vertical temperature structure over large areas appears to be an appropriately instrumented light plane. With this, one could record a vertical temperature profile up to a height of 1,500 meters within 10 minutes. Within only an hour, one would have 4 to 5 represen-tatitive profiles over a congested area. Along with the position of inversions, one would also have the stability of all the other layers. These are aids so that something can be said about the turbulence occurring and about turbulent diffusion.

At present there is no possibility of establishing the existence of low inversions. Neither can we conclude anything about the stability of the vertical temperature layering from the temperature profiles, but only indirectly through certain routine meteorological measurements such as wind strength, degree of cloud cover, and simple estimates of the radiation. This situation is very unsatisfactory, although surprisingly good simulation results can be obtained with this method. This is because practical diffusion experiments had been done previously under conditions correlated with the simple scheme for characterization of stability classes. Literature in this relation includes [7, 8, 9].

We shall demonstrate the importance of inversions for air quality maintenance problems with some simple examples. Let us consider a congested area covering the area F. Let the total emission of the area, for some air pollutant, be Q, and assume that we are dealing with continuous emission. In the case of a weather condition with weak wind, this amount of emission is placed in a cylindroidal volume. Let this volume be bounded by an inversion at the height H. Let the pollutant be able to distribute itself rapidly enough in the vertical dimension so that we have a height-independent concentration distribution. If the concentration S_0 at the ground is given at time $t = _o$ (starting time), and, so, also in a vertical column of cross section 1 m^2, then the concentration S grows with time according to the formula

$$S = S_o + \frac{Q}{FH} t$$

This rise is inversely proportional to the height of the inversion, and we can see that with low-lying inversions, there can be threatening concentration rises in relatively short time spans.

If we take the following as a numerical example: $F = 250 \text{ km}^2$, $Q = 25$ tons/hour and $S_o = 0$, then we obtain

$$S = 100 \frac{t}{H} \quad [\text{mg m}^{-3}]$$

if the inversion height is given in meters and the time t in hours. If the inversion is at the height of the upper limit of the planetary boundary layer (1,000 meters) then the concentration rises at the rate of 0.1 mg m^{-3} per hour. If the situation is maintained for 10 hours, we get an average load of 0.5 mg m^{-3}. With an inversion height of 200 meters, the hourly rate of concentration rise is 0.5 mg m^{-3}. Then we see that in two hours we have already arrived at the situation of an average load of 0.5 mg m^{-3}. This example may suffice to show the importance of including inversions in models [5].

2.3 Problems of physical and chemical conversion of foreign substances during transport in the atmosphere

Until a short time ago, sulfur dioxide was used almost exclusively as the controlling substance for the solution of planning problems, because of the well-known injuries to the biosphere from high sulfur dioxide concentrations. One example of this is the method for the determination of minimum smoke stack heights on the basis of the maximum SO_2 concentrations attained at the ground. In these calculations, it was realized early that overly high ground immissions are predicted under certain conditions because of the many conversions of SO_2 in the atmosphere during transport. In the lack of a reliable theory of the physical-chemical conversion processes for sulfur dioxide, then, all the concentration decreases in the atmosphere caused by conversions were considered, using a half-value time T, in the form of an exponential decrease with the travel time $t = x/U$. The travel time for an air quantum is the time which it requires to go from the site of emission ($x = 0$) to a location which is a distance x away. This time depends on the average wind velocity U at the height of the drifting air quantum. An exponential decrease with the travel time, then, means

$$s \sim \exp\left[-\frac{\ln 2}{T}\frac{x}{U}\right].$$

If the travel time $t = x/U$ agrees with the half-value time T, then the concentration has diminished to half as a result of conversions alone. The following simple table shows the distances x at which the concentration appears reduced to half, for various half-value times T and different wind velocities U:

U / T	10 min	30 min	1 h	3 h	6 h
2	1,2	3,6	7,2	21.6	43,2
5	3,0	9,0	18.0	36.0	72.0
10	6,0	18,0	36,0	108,0	216,0
15	9,0	27,0	54,0	162.0	324,0
20	12,0	36,0	72,0	216,0	432.0

U in Meter/sec
x in Kilometer

A 50% concentration decrease caused by conversions must unconditionally be considered in all model calculations. Now according to the table above, whether or not the conversions prove important for modeling depends on the half-value time T, the meteorological conditions (U) and the spatial dimensions (x) of the region. An example may clarify this: The city of Bremen has a northwest-southeast extent of 40 km at the most, and a southwest-northeast extent of 20 km at the most. The frequency distribution of wind direction and wind strength states that for the predominant number of hours in a year, winds flow at a velocity of 10 m/sec over the city out of the southwest. The extent of the city in this direction is only 20 km. For these conditions, we find from the table that the conversion processes would need to be considered only for half-value times below 30 minutes. At half-value times of about 3 hours, a value presumed in the modeling of the immission conditions for this city, the conversion processes need not be considered. The conditions are considerably different in larger population centers, where it is not only the conversion process for SO_2 but also those for all the other chemically reactive substances, with their different half-value times which must be considered in modeling.

The necessity of model simulation of transmission, with consideration of physical and chemical interactions between the various foreign materials in the air, on one hand, and with the permanent gas components of the air or with its water vapor and water content on the other hand, was recognized in the United States relatively early. It was stimulated particularly by the "smog" phenomenon in the Los Angeles basin. Here we always deal with long reaction chains which begin with the originally emitted gases and lead through physical and chemical interaction to the occurrence of secondary substances. Only in the rarest cases do these themselves remain stable. Even the chemical career of sulfur dioxide has not been followed up in all the necessary details. This explains the fact that half-life values between 10 minutes and several hours have been reported for SO_2 [10]. These conversion processes are usually sinks for SO_2 in the atmosphere, in that it is removed from the air by these processes.

This occurs, in one way, on purely chemical paths through binding with the nitrogen oxides and the hydrocarbons, with or without the action of solar radiation. The resulting chemical substances then change into other substances. Absorption of SO_2 in water droplets, on metal oxides (lead, iron, vanadium) and on aerosols of certain solution character, as well as washing out by rain, and many others, are effects which are also sinks for sulfur dioxide. Rarely does a SO_2 source develop in the atmosphere through the photochemical conversion of hydrogen sulfide. It is characteristic that almost all the processes named depend very strongly on the temperature, the air pressure, the air humidity, and the solar radiation. These parameters determine primarily the reaction rates of the chemical interactions. These, for instance, can be doubled by temperature changes of 10°C. Obviously, all the reactions depend on the existing concentrations of the participating substances and on the spatial distribution of the meteorological parameters.

What has been said about sulfur dioxide applies similarly for all the other chemical substances found in emissions from industry, traffic, and house fires. Only recently, on the initiative of the Ministry for Labor, Health, and Social Affairs of the State of Nordrhein-Westfalia has there been work on a complete register of all the emitted substances which can be detected in the Cologne area [11]. All of the chemical substances established in the emission collection, some of which are not inferior to sulfur dioxide in danger or degree of stress (odorous materials), and which arise in considerable amounts from low sources, lead to the fact that the entire planning strategy, based on SO_2, must be tested. Additional control substances will appear in planning problems. Most of these will be substances which are subjected to physical and chemical transformations in the atmosphere and/or at the earth's surface much more than SO_2. This makes the problem of model simulation of air pollution situations extremely complex.

For every individual substance we must not only find and solve a transport equation, but also an equation indicating what amount of this substance appears, in what time, from the chemical interaction with perhaps many other substances. These relations, called reaction equations, are as yet known for only a very limited number of reactions. They are also known only in [illegible] empirical form, with the use of coefficients which can only [illegible] determined incompletely from laboratory experiments (or from idealized theories). In particular, the hydrocarbons in the atmosphere lead to hundreds of individual reaction steps which end in the production of dozens of new substances in the atmosphere. These were not originally present in the emissions (primarily from traffic). All this goes on under the controlling action of continuously changing meteorological parameters, as the reaction coefficients depend sensitively on them; but, the effect of air pollution on the distribution of the meteorological parameters can often be established clearly (especially in the case of the effect on solar radiation and the meteorological secondary effects which it produces). These then affect the distribution and the mutual reactions of the chemical substances. The situation becomes particularly critical in cases where a weather condition with weak wind and exchange is linked with development of a low inversion. Under these conditions there are strong spatial variations of the meteorological parameters, and there arises a complex picture of the air pollution, with high concentrations and rapidly occurring chemical reactions which we cannot clearly conceive. At present, model simulation of the spread of chemically and photochemically reactive substances is very much at the front of international research because this is one of the most pressing problems for the future.

2.4 Mathematical problems in model simulation

In the mathematical simulation of air pollution situations, no problems occur which would appear mathematically other than as analogous problems of theoretical physics. As there, we calculate a deterministic prediction for later times from knowledge of the initial conditions, with the help of model equations in the form of partial differential equations, considering boundary conditions. In the sentence just formulated, however, there is concealed quite extraordinary difficulty in applying the statement of mathematical problems to the existing problems.

1. For the purpose of a short-term prediction and the related control strategy, we can in no way determine an initial state of the concentrations of foreign substances in the atmosphere of the region of concern which is described with mathematically adequate accuracy. Usually there are only measurements of ground immissions, with no measurements from the higher air layers. Mathematical and physical methods can lead only to a probable initial distribution of the spatial concentrations, and after studying the sensitivity of the predicting equations we must understand clearly how uncertainties in the initial conditions affect the resulting immission prediction.

2. The model equations in the form of partial differential equations represent only a more or less good mapping of natural conditions onto the conceptual system of mathematical physics. Many effects, such as atmospheric turbulence, cannot be described accurately in the language of mathematics. This fact introduces more uncertainties into the immission prediction. But even with optimal mathematical formulation of the natural process, the solution of the mathematical equations has such a difficult form that we must refer back to approximate solutions. These are also

linked with production of uncertainties in the immission prediction.

3. The mathematical formulation of boundary surface conditions, as at the natural surface of the earth with all its small-scale irregularities, is likewise quite difficult and cannot be done with mathematical exactness.

For the reasons given, we cannot expect that we will ever develop mathematically exact deterministic prediction models in the field of air quality maintenance, in the sense that exact initial and boundary conditions will produce unambiguous immission predictions which agree with conditions in nature on the basis of exact model equations. In this area, as elsewhere in meteorology, one must become accustomed to the idea that we can only expect statements of more or less high probability. For this reason, mathematical statistics, and still more the theory of stochastic processes have been gaining dominant importance in the field of air quality maintenance along with physics and meteorology. For anyone concerned with the propagation computations practiced today this fact is not new. The generally known formulas for the propagation of smoke plumes are results of the statistical theory of turbulent diffusion. The first model for the immission climatology of a city (Bremen) [5] is a purely statistical one also. It is solely statistics of immission fields which are computed from the statistical properties of the smoke plume spread around isolated sources and from the statistics of meteorological propagation conditions. Thus we cannot expect that an individual measured immission value will agree with a statistically determined one. Naturally, these facts have the most serious effects on the quality of short-term immission predictions. They make it difficult to make decisions to carry out the control strategy. Still, there is no doubt that we can take reasonable control measures on the basis of predicted probable immission situations for which the error limits are given.

First, though, the development of the mathematical model for the simulation is very much in the foreground of research. For any problem which might occur in the field of air quality maintenance, this model should be able to simulate optimally the conditions in nature. After all that has been said before, it is not to be expected that a universal model can provide the desired answers to all questions in the field of air quality maintenance. More models must be developed just for the spread of a single smoke plume, depending on the terrain (topography) in which the spread occurs, and on whether or not chemically reactive substances are emitted. The type of emission, whether constant or variable with time, is also of decisive influence on the type of model to be developed. If we continue to the problem of modeling the immission conditions for a city or for a populated area, then far more mathematical problems occur due to the spatial dimensions and the more widespread emissions than in the case of the single source. Topography and the time dependence of the emissions are not the only problems. There are also the problems which arise in the mathematical treatment of the area sources, particularly those which occur because of the meteorological differences within the area. The interactions between the air pollutants and the meteorological parameters also gain more importance, forcing us to solve the meteorological prediction problem simultaneously with those for the spread of the air pollutants. At present, this problem is one of the most difficult in predictive meteorology. Here we must predict not only the large-scale distribution of the meteorologic parameters, but the state of the structure of the atmospheric turbulence and the detailed vertical distribution of the temperature (for the stability of the layering and particularly of inversions). This must be done with full consideration of the interactions between the air pollutants and the meteorological parameters. If we have a case in which chemically reactive substances mix with each other, then the mathematical difficulties are multiplied. Along with the previously mentioned meteorological equations, we must then solve equations for each gas component as well as for the various reactions simultaneously with all the other equations.

3. THE PRESENT MATHEMATICAL-METEOROLOGICAL MODEL FOR THE SOLUTION OF EMISSION- AND IMMISSION-ORIENTED PLANNING PROBLEMS AND FOR AIR QUALITY MONITORING

In Chapter 1, we stated the pressing necessity of early initiatives to develop control strategies to maintain immission limits always and everywhere within industrial complexes, to develop immission-oriented city and regional planning measures, and for the careful observation of climatic changes due to air pollutants. After that, we showed that all these problems can be solved only with the aid of reliable immission predictions. The prerequisite for such predictions is the presence of reliable mathematical-meteorological diffusion models. Their use requires the presence of detailed emission registers. On this basis, we discussed the scheme of an internally programmed computer control strategy to solve the problem of constant maintenance of the immission limits. We explained the concept of immission climatology, which has great importance for determination of the basic immission load and for the solution of many city and regional planning problems. It was not specifically mentioned that the model computations also open up the possibility of reducing drastically the number of measuring sites in the air quality monitoring systems. With the models, we can not only undertake a rational stragetic planning of measuring nets, but also, the models are able to use the computer to simulate measurements between the stations and to interpolate.

In Chapter 2, we compared these optimistic perspectives with the difficulties which still today stand in the way of realization of the potentials indicated. We still lack a satisfactory theory of atmospheric turbulence and of turbulent diffusion. We do not yet have sufficient command of the problems of flow over topographic unevenness, and in particular we can say nothing accurately about the resulting turbulence and turbulent diffusion. The problem of theoretical treatment of smokestack superelevation under all characteristic meteorologic conditions is still unsolved. We have only empirical relations, some of which give results deviating seriously from each other.

Many important problems are yet to be solved on the side of meteorology. The general prediction problem for the structure of the planetary boundary layer must be considered as insoluble for a long time. The case is similar for thermal convection, for weather conditions with weak wind and exchange, and for the fine structure of the wind fields in both the horizontal and vertical planes in large congested areas. The demonstrated importance of low inversions on the immission situation also makes the prediction or the systematic investigation of inversion weather conditions seem particularly important.

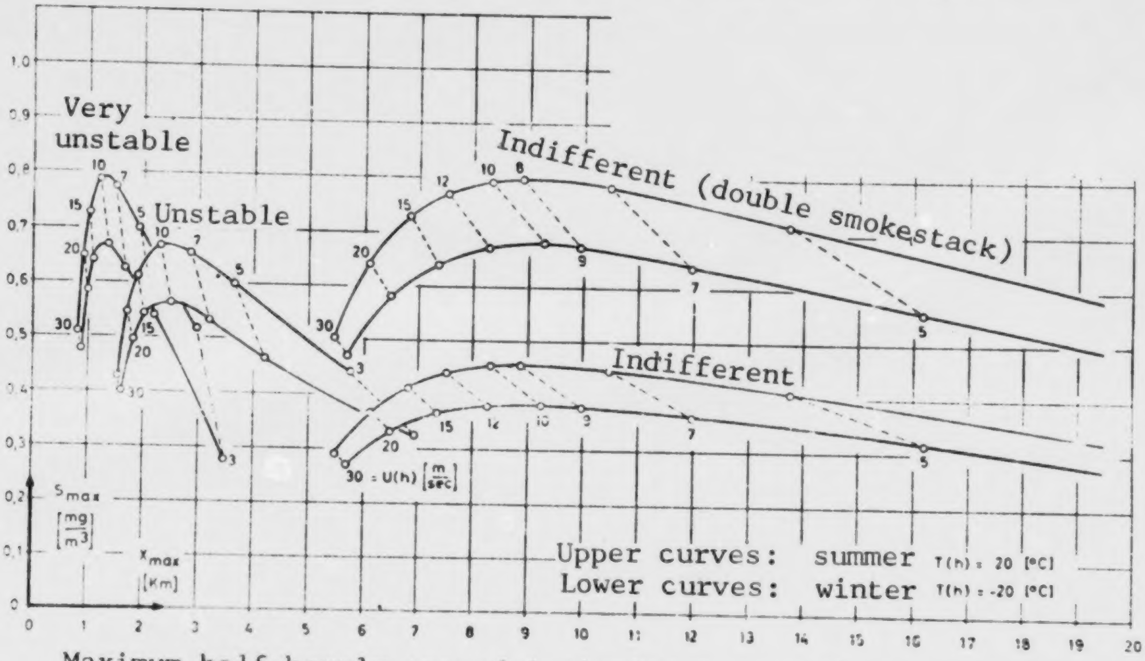
On the problem of the spread of chemically and photochemically reactive substances, we could make only its nearly hopeless complexity plausible. Correspondingly, even today there are hardly any useful trial solutions for a model simulation. Here we refer only to the summary report [12].

In spite of these and other mathematical problems, theoretical meteorology has been intensely concerned with model simulation of air pollution situations for more than 20 years. The pioneering contributions of O. G. Sutton [13], F. N. Frenkiel

[14] and F. Pasquill [15] are generally well known. These authors laid the foundations for the so-called propagation computation which is in practical use today. The most important applications and further developments in the German Federal Republic have originated since 1957/58 in the VDI Commission on Maintenance of Air Purity. A working group of the "Theory of Propagation" subcommittee worked up the bases for the VDI Guideline 2289 for determination of minimum smokestack heights [1]. Immediately after the guideline was finished, the author took up work on the problem of the immission basic load, which appears there. It was ready for programming in 1962.

3.1 Model to solve the problem of minimum smokestack heights

The problem of minimum smokestack heights belongs in the group of problems of city and regional planning. According to Figure 1, it is in the planning control loop. According to what has been said before, then, the planning strategy to determine minimum smokestack height for a single planned emitter goes as follows: The emission register consists solely of the data for the intended plant. These are, along with the geographical position and the construction height, primarily the source strengths for the individual pollutants and data needed to calculate the smokestack superelevation. All the relevant meteorological data, divided into wind direction, wind strength, and propagation classes, together with regional, primarily topographic, data, make it possible, using the optimally valid model for the conditions of interest, to compute a ground immission field for every combination of the meteorological parameters, assuming constant emission and the development of a stationary linear smoke plume. From this calculated ground immission field we can calculate the maximum ground immission as well as the distance at which it occurs. Both values depend on the wind velocity, on the class of propagation, on the air temperature (which is included in determining the smokestack superelevation) and on the wind direction, if topographic effects come into play. Figure 4 gives an example for the relation s_{max}-x_{max} as a function of the windstrength U at the height of the smokestack opening, the propagation class, and the air temperature (upper curves for summer, lower for winter) in the case of the specific system: construction height 220 meters, source strength 10 tons per hour. The case of a double smokestack of this type, with 100 meters separation, is plotted only for the "indifferent" propagation class [16]. With this example we already see most of the problem raised on the determination of the minimum smokestack height. If we assume the most



Maximum half-hourly ground immission s_{max} and corresponding source distance x_{max} for a 700 MW unit ($Q=10\left[\frac{t}{h}\right]$) for various atmospheric conditions as well as for a combined 1,400 MW system ($Q=20\left[\frac{t}{h}\right]$) and "normal" atmospheric conditions.

Figure 4.

unfavorable conditions to evaluate the intended plant, then for very unstable atmospheric layering, for a wind velocity of 10 meters/second, and for summer temperatures, we would find a maximum half-hour ground immission of some 0.8 mg/m^3 at a distance of only 1 km from the source. This would exceed by 0.3 mg/m^3 the MAC$_k$ value for SO_2. This situation would prevent issuance of a license for construction of the intended plant. The person proposing construction could now concern himself more closely with the meteorology of the district in question, and might establish that such unfavorable weather conditions are extremely rare during the year, and that, in comparison, there are "almost always" indifferent layering conditions. Even in the summer, and for all wind velocities, these would insure that the maximum ground immissions he produces would not exceed the MAC values. In addition, they would occur at the large distances of 10 to 15 km from the source, where, with the prevailing wind conditions, they would strike land which is not built up and not used agriculturally. The controlling body could not ignore these arguments. On the basis of a mathematical-meteorological diffusion model they would establish suitable control strategies for this plant so that the emissions of the intended plant could be reduced suitably in the predicted unfavorable weather conditions.

Obviously, the frequency of the occurrence of "favorable" and "unfavorable" weather conditions plays a decisive role for the case depicted. It is theoretically possible to conceive of weather conditions for which there would be no excesses over the MAC at smokestack construction heights of perhaps one tenth that of the planned height. These, then, would be "favorable" weather conditions. With "unfavorable" weather conditions, perhaps twice or three times the height would still not be enough to keep from exceeding the MAC. If one were to specify the technological emission values of the plant, then with model simulation of the transmission for this plant, one could determine from the frequency distribution of the meteorological situations a matching frequency distribution for the required minimum stack heights which would guaranty that overstepping the MAC values would be prevented. For the plant on which Figure 4 is based, these heights would be between 80 and 400 meters. Economic considerations also enter at this point. If one saves the building cost for a high smokestack, then, due to the frequently occurring emission limitations, one must count on comparable loss of production. If one builds a very high, very costly smokestack, then there will seldom be production losses due to a necessary emission limitation. The economic optimization process to be applied can be played out without difficulties using a propagation model. We can even include many other parameters, such as the outlet temperature or the outlet velocity of the smoke gases, in the optimization process. The whole acceptance process can be played through in the computer so that both the interest of the public and that of the builder are considered in a balanced way. At present, though, we are still far from this goal. Some reasons for this are the following:

In most cases, an newly planned plant will not be the only one in an otherwise emission-free countryside with a radius of 20 km around the source. There will already be an abundance of other sources, generating a corresponding preliminary load (basic immission load). The entire licensing procedure depends decisively on this preliminary load. This fact has long been considered in places concerned with licensing of plants of the type depicted. Furthermore, the TI Air [1] offers guidance on the technological determination of this preliminary load (see also [2]). For reasons presented previously, however, the author took the side of model simulation of the basic immission load also, simply because it is too difficult and costly to determine the necessary spatial fine structure of the basic load fields by measurement. It was also suggested that these change continuously because meteorological conditions vary from year to year, and because of the addition of new emitters, so that no standard can be developed to solve planning problems. Before applying models to determination of minimum stack heights, then, the problem of the basic immission load must be solved in a satisfactory manner. This was first done in an examplary manner for the city of Bremen [3, 4, 5], where it was also demonstrated how a rational combination of theoretical modeling with tests of the theoretical results by measurement opens up the possibility of subsequently "calibrating" the model on the basis of the measurements. This appears to show the future direction of basic load determination.

Other problems for the model simulation of minimum stack heights have already been mentioned. These concerned our ignorance in the area of theoretical description of the atmospheric turbulence, the vertical and horizontal wind structure, the thermal stability (inversions), the thermal convection and the influence of the topography, along with the chemical changes and the absorption within the atmosphere or at the earth's surface. Unfortunately, because of the urgency of the solution of air pollution problems, we no longer have time to solve the problem which has been raised with completely satisfactory scientific accuracy. Therefore, we can deal only with pragmatic solutions which, we hope, can serve to answer the problems posed with sufficient accuracy, although the concept of "sufficient accuracy" can be the subject of endless arguments. Nevertheless we must decide, and this is universally done in the following manner (see in particular the review [17]). The course of the meteorologic parameters, which is continuous in time, is made discontinuous by classification into a finite number of wind direction, wind strength, and propagation classes, with the lengths of the time intervals specified (usually hours), for the classes in which the meteorologic parameters are found. We also give up the time sequence of these successive discontinuous states of the atmosphere – then, for a long period (month, heating period, year, decade) the frequency one classified combination of parameters is encountered. A typical statement of this type is, for instance: During the 8,760 hours of 1969 there occurred 400 hours in which the wind direction was between 240° and 250°, the wind strength was between 7 and 9 m/second and the propagation parameter was in class 4 (indifferent), without consideration of the time relations. Such a combination of meteorological parameters determining the transmission is a weather situation. This is taken to be constant during the selected time (hour). The same applies for the source strength, which is set constant. In all, steady state conditions prevail during the time interval, and it is presumed that a steady smoke plume also develops to its full length and width. This smoke plume must have a linear axis parallel to the ground, where the ground is presumed to be flat. The irregular nature of the earth's surface and the spatial variation of the wind field which it causes are also excluded, as is absorption at the surface of the substances emitted by the source. Extended field experiments [15] under conditions which are rather similar to those just described led to the result that the spatial distribution of the waste gas concentration can be described, on the average, by a biaxial Gaussian distribution in planes perpendicular to the wind direction. If the stack superelevation is known, this concentration distribution is determined only by an appropriately vertically averaged wind velocity U and by the standard deviations σ_y and σ_z of the Gaussian distribution in the directions perpendicular to the wind direction. These standard deviations (also often called dispersions) depend on the state of the planetary boundary layer, that is, on the turbulence and also on the stability of the vertical temperature layering. In view of the abundance of literature on this model for mathematical-meteorological simulation of the spread of a smoke plume in the lee of a stationary point source, we need no further discussions here. A discussion of the formulas and solutions widely accepted today appears in [17] in relation to reasonable applications.

The principal deficiency of this model for a single source is in the determination of the standard deviations from empirical field experiments and in establishing an average wind velocity representative for the propagation process within the planetary boundary layer. Field experiments under idealized conditions yield standard deviations which are often not sufficiently representative for the area of application, such as a city. Also, the assignment of the measured standard deviations to routinely done meteorological observations of wind, cloud cover and radiation is subject to great sources of error. Something similar applies to the selection of a representative wind velocity from ground wind measurements alone. This, along with the previously mentioned difficulty which arises in the empirical determination of the smokestack superelevation, makes the previously applied propagation calculation appear to be merely an empirical theory applied to the most urgent practical problems. Its theoretical foundation and verification are still lacking.

The practical utility of this model, which still appears so incomplete, is unargued today throughout the world. There is no country in which this model is not being applied in the emission and immission-oriented planning. In the Federal Republic, the statements of the model have had a decisive effect for many years on the course of the licensing procedure in the form of the TI Air [1], using reasonably simple meteorological statistics. (Only a single propagation class and only a small number of wind strength classes are used.) General opinion seems to oppose trusting the accuracy of the method for planning purposes; but, severe doubt will always be raised if we attempt to simulate actual ground immissions with the help of the model. The model, however, is not provided for that purpose at all. It represents the statistical result of many individual experiments, of which each individual one can be classified only as rare and incomplete in the scheme to describe the average conditions by formulas.

Even within the structure of this simple theory for the propagation of a steady smoke plume, improvements are still possible in the direction of including effects which have not yet been considered. These concern, among others, the case of weather conditions with weak wind and weak exchange. For wind velocities above some 2 m/sec, the turbulent diffusion in the direction of the wind becomes so insignificant, in comparison to the transport by the wind, that only the transport need be considered. This has its consequences in a particularly simple form of the concentration distribution. Transport by the wind is linked with the travel time of an air quantum, $t = x/U$. Turbulent diffusion is linked with the coefficients of turbulent diffusion, which assume values around 1 to 10 m^2/sec. With K as a diffusion coefficient, a characteristic diffusion time t_D to cover the distance x is given by $t_D = x^2/K$. The assumption mentioned above can be justified only for the case in which t is very much smaller than t_D. This condition is met if U is very much larger than K/x. In this case, we must select the characteristic "scale" of turbulence for x according to Figure 3. This is between 1 meter and 100 meters. From the theory of turbulence, we know also the Richardson relation for the relation of the diffusion coefficient K to the "scale" of the turbulence: $K = 0.2\ x^{4/3}$. Now, as a condition for the approximation under question, this states that the wind velocity U must be very much greater than $K/x = 0.2\ x^{1/3}$. For light turbulence, $x = 1$ m, $K/x = 0.2$ m/sec. For strong turbulence, x = 10 m, K/x = 0.43 m/sec. For conditions which are already in the range of transition to thermal convection, x = 100 m, K/x = 0.93 m/sec. Thus, how great the wind velocity U must be depends very much on the state of turbulence in the flow if we are to justify the assumption that the turbulent diffusion in the wind direction is negligible in comparison to the transport by the wind. For light turbulence, we can accept this for U greater than 1 to 2 m/sec. For strong turbulence we must already require that U be greater than 2 to 4 m/sec. At the beginning of convection, U must, theoretically, be greater than 5 to 10 m/sec. Conditions with weak wind, however, are particularly interesting. These occur relatively often in the interior. They are, for instance, fall foggy weather conditions with very slight turbulence and weak wind. Here the model equations are certainly no longer applicable. In summer high pressure weather conditions, the case of strong convection is realized with high irradiation. But at the same time, the wind velocities are very often below the value of 5 to 10 m/sec stated above, so that the model is also not applicable under these conditions. Because of the frequency of these two limiting cases, development of a propagation model for low-wind or windless weather conditions is a very urgent one. An early trial solution was undertaken in [18], where the propagation in the lee of a point source was studied for the case in which the smoke plume axis has an arbitrary form. This includes the case of a smoke plume rising vertically to an equilibrium height because of thermal buoyancy, and gives the development with time of the concentration field under an inversion in a calm. Figure 5 shows the conditions 30 minutes after the beginning of emission from a source 100 m high with a source strength of 360 kg/hr and a stack superelevation of 100 m, as calculated from the exit velocity of the smoke gases, under an inversion which is 24 cm from the ground (1).

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(1) Translator's note: Figure 5 indicates that this figure is a typographical error, and that it should be 240 m.

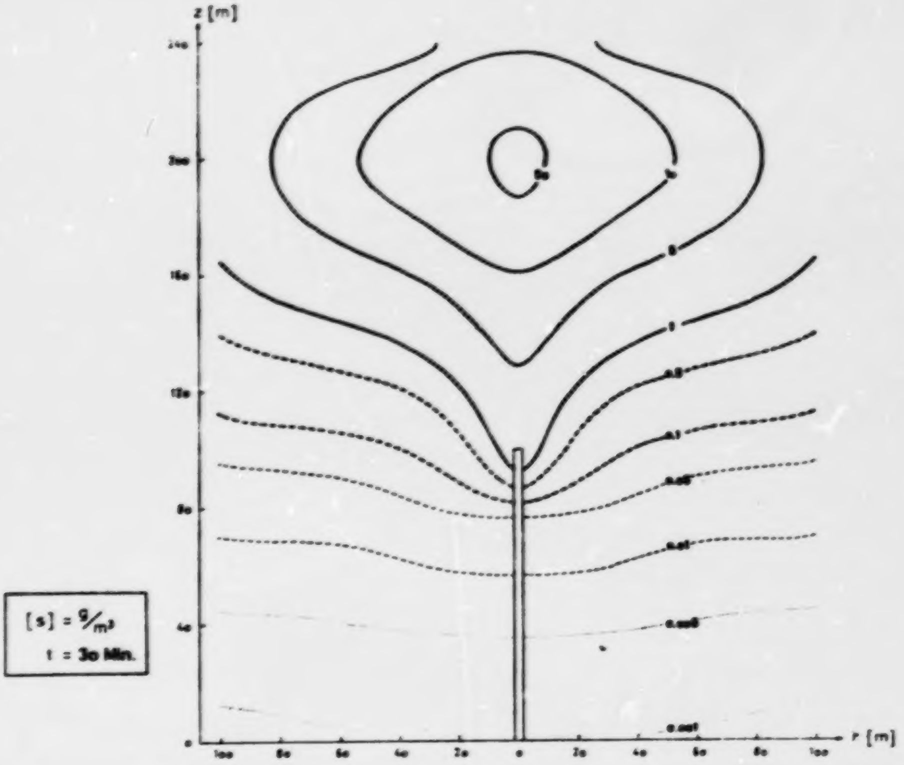

Figure 5. Spread of a smoke plume rising vertically under an inversion, 30 minutes after the beginning of the emission.

Under these very hazardous conditions, concentrations of 1 mg/m^3 occur at the ground after even this short time. If this situation is maintained for many hours, there would be theoretical concentrations of the magnitude of g/m^3, although these depend greatly on the diffusion parameters used. But we have no data for these conditions. Standard deviations $\sigma_x = \sigma_y$ and σ_z have not yet been determined for calm weather conditions.

One often observes smoke plumes rising vertically; but beyond a certain height they are deflected by a wind which exists there. Then they spread more horizontally and vertically as in an atmosphere with stable layering. Here, we must treat the spreading process in the calm layer separately from that in the upper layer, and the model mentioned provides for the manipulation. Other cases are related to the suppression of smoke plumes by some sort of effect which has not yet been accurately studied meteorologically. This also applies for smoke plumes which have a smokestack superelevation due to their thermal buoyancy. These cases also belong in the statistics for the determination of minimum stack heights, and can be modeled by means of the results from [18].

Much effort has been devoted to the development of supplemental aides to VDI Guideline 2289 which is the basis of the TI Air, among others, so that the ground topography can be taken into consideration. The results are reported in [19]. There still remain extensions of the model for the case of emitters in valleys. Here we find calm particularly often, and particularly stable layering is realized. But even with vigorous air movement, the wind structure in the valley area is often very complex. In the summer, there are also thermal circulations due to the development of catabatic and anabatic winds in the sloping regions. In this relation, it is interesting to mention that because of the difficulties of mathematical simulation of smoke plume spread over irregular topography, researchers are seriously developing physical simulation in the wind tunnel or with flow in a water tank [20, 21]. These attempts are very promising for the treatment of individual cases; but it will not be possible to get aids for the establishment of guidelines this way. Nevertheless, intensification of research in this sector could pay off well. The results obtained from it could probably not be similated in any way with a mathematical model, at least, not if we are dealing with real topography.

In order to apply practically the mathematical-meteorological simulation of the spread of smoke gases in the lee of an isolated single source, we still need to establish the following. From the character of the model, it should be part of immission climatology. Therefore, it should not be used for temporal predictions in the sense of a short-term prediction. It is not possible to simulate time-dependent immission situations by means of a sequence of statistical immission distributions which were in addition obtained on the assumption of steady conditions. Such attempts have always failed. The investigations in [22] may give one example. There was in this case an inclination to reject the mathematical simulation model entirely because of the insufficient agreement between measured time series of immissions and those computed in parallel from the mathematical simulation model. In this respect, the author was able through long personal discussions to convince F. Pasquill that only an agreement of the temporally unordered frequency distributions of the immissions can be expected, and that he should suggest such an evaluation of their data to those authors. The results later reported by Pasquill [23] were a distinct success for the method of mathematical simulation.

Today, the point source model has matured so that its use for determining minimum stack heights is no longer in question. Only the meteorological "statistics" (the calculation is hardly based on any) used in the TI Air and in the original VDI Guideline 2289 need improvement. This problem has been discussed productively in the VDI subcommittee "Theory of Propagation" and has led to development of a new concept of the guideline (First Draft, [24]). The basic idea is the same one which has already appeared often in relation to the discussion of an immission climatology. The frequency of the occurrence of "favorable" and "unfavorable" weather conditions finally decides the construction height of the smokestack to be newly erected. It is apparent that the propagation conditions are more favorable in the area of the North Sea coast than in the congested area of Frankfurt, where higher stacks are needed than in the coastal area.

3.2 Models for the immission climatology of industrial concentrations

We have often emphasized that a simulation of the immission climatology of cities or populated areas is of decisive importance for any immission-oriented city and regional planning. Even the relatively simple problem of minimum smokestack heights is essentially insoluble without knowledge of the immission climatology of the complete region, if necessary. Planning of a single smokestack is already an immission-oriented city-planning measure. Usually no serious change of the immission climatology occurs from a single new stack. It is different when new industries move in or when new housing areas with individual heating systems are permitted. Also, the development of the traffic system, the expansion of a harbor, conversion of heating to other fuels are all processes and changes which often have a quite decisive effect on a change in the immission climatology of the region. If one takes serious thought about the area of air quality maintenance, one is forced to be clear, before carrying out the planned changes on the emission side, on what effects they will produce on the immission side. This is possible solely on the basis of an immission prediction, in which the planned emission changes serve as the model input. This has been emphasized again and again in these considerations.

The first complete model for the immission climatology of a city, based on an emission register, was conceived after the conclusion of work on VDI Guideline 2289. It was directed toward calculation of the basic immission load for 1961/62. The 1965 model computations were done after provision of the data for the 1963/64 emission register, and the first publication appeared in 1966 [3]. This was translated shortly thereafter in the Air Resources Laboratory of the ESSA in Cincinnati, Ohio. Subsequently, use was made of the method of emission register collection, just as it was first applied in Bremen. A model with the same information content as that developed for Bremen, verified by a directed measuring program, has not yet been found in the literature. Thus, it seems justified to describe the basic ideas and the practical problems related to the model developed for Bremen rather more extensively than has been done before.

In the following, we shall again make use of the statements in the block diagram of Figure 1, which we pictured as a conceptual scheme for the starting point at the beginning of the work. The problems described in Chapter 2 were also known in their full extent. In order to be able to carry out a first experiment in the direction of mathematical-meteorological simulation of immission climatology and of the basic immission load, it was important to find conditions which would justify application of the available theoretical solutions. It was also necessary to find a city which considered itself able to produce an emission register. It was just this problem of an emission register which proved insoluble about 1962/63. We had originally thought about modeling of the entire Ruhr area with a relatively simple model. But although there were already extensive emission collections in this area, we could not consider establishing an emission register of the kind needed; and furthermore, there were legal reasons against providing emission data for research purposes. A private attempt to find an American city with an available emission register also failed. It was generally said to be impossible to establish an emission register for sulfur dioxide (which was then at the center of all interest) divided up according to industrial sources, home heating sources, and trade sources, with the necessary accuracy. Provision of the necessary support to carry out such a modeling test initially appeared impossible also. This was realized only after convincing a responsible member of the Hessian Ministry for Economics and Transportation (R. R. Caroselli) and through support by colleagues (F. Wipperman, Darmstadt). In addition, the responsible authorities of the city of Bremen declared themselves ready to attempt to set up an emission register for sulfur dioxide. To do this, the individual sources were covered by means of a questionnaire or by calls from an official of the Trade Supervision Office [3]. This method is still used today. Home heating emissions were covered differently. In Bremen, home fires were considered an area source emission. This was determined on the basis of the area use plan for the city (the number of inhabitants, the dwelling units, and the size of the inhabited area were known for each numbered district) and from the amount of fuel used for home fires during a heating period. This gave an average SO_2 emission per dwelling unit and hour of 8 grams. The initial values in this calculation were: Fuel per heating period (heating period = 6,100 hours); Coal, 328,000 tons; Oil, 124,000 tons. The total amount of fuel per hour is then about 74 tons. From the sulfur content of the coal and oil, we obtained an average SO_2 emission of 1.6 tons per hour for home fires. With about 200,000 dwelling units, then, we get the value of 8 grams per dwelling unit and hour. We can see that this is a plausible value if we work backward to the heat which this provides per dwelling unit. If we assume an average sulfur content for the fuel, we get an associated SO_2 emission [17] of x%. Conversely, the SO_2 emission of 8 g/hr corresponds to a fuel quantity of 8/x kilograms per dwelling unit and per hour. If we suppose a volume of some 200 m^3 per dwelling unit, we arrive at a fuel quantity of

8/200x kg/hr. Based on a heating value of 6,000 kcal/kg, this yields, as the equivalent amount of heat, the value 48,000/200x = 240x $kcal/m^3hr$. Now we must also consider the efficiency of the heating system and the SO_2 output x in % to obtain the corresponding amount of heat. This varies between 50 and 100 $kcal/m^3hr$. These values, which correspond to practice, are equivalent to a SO_2 output of about 10 g per dwelling unit and hour. The emission registers which are now established in various regions [17, 11] go into much more detail.

Now if we know the spatial distribution of dwelling units, at the same time we know the average house fire emission. For purposes of immission modeling we cannot avoid relating the home fire emissions to area units of certain size. We have recently selected an area size of 100 x 100 meters [11]. At the beginning of the modeling work in Bremen we had used a size of 1000 x 1000 meters, and later 500 x 500 meters. The choice of the area size depends decisively on the spatial variability of the housing density, and thus on the house fire emission. Through dividing up the regions into area elements we intend to represent the spatial variability of the emission conditions in simplified form so that we can assume an average, homogeneous area emission for each area element. The extreme case on one side would be the assumption of a constant average emission in the whole city area. Here we would ignore any spatial differentiation of the emission, and it cannot be expected that modeling of the immission conditions would give very detailed results. We would have the other extreme case if we tried to include accurately the emission of each apartment house and each separate house. Aside from the fact that such a detailed emission collection would be too expensive to carry out, we would also have to undertake more extensive investigation of the flow structure in the areas of influence of the buildings and also of the time variability of emission and of meteorological conditions. As Figure 3 shows, in meteorology there is always a certain relation between the spatial and the temporal "scales" for the phenomenon under consideration. There is an analogous situation for emission in the field of air quality maintenance. Industrial emission usually has a very large time "scale", because it is largely continuous. The space "scale" can be characterized by the mutual separation of the point sources. Emission from home fires, in contrast, shows a pattern through the day, with the effect of air temperature superimposed on that. The range of the time "scale" will extend from about one hour to several days, and will depend not only on the time of day but also on the meteorological conditions. The matching spatial "scale" would be between 1 km and more than 1000 km, on the basis of the meteorological influence. Here two spatial "scales" appear for the home fire emission field: one length to characterize the average spatial variability of the emissions, and one length which indicates the dimensions of the entire region (city, congested area). It is very difficult to say generally what area element division one should choose for home fires. For cities which are not too large, where we must choose a time "scale" of about one hour in order to consider the variation of home fire emissions with time of day, meteorological reasons would give a space "scale" of a kilometer. This gives an area size of 500 x 500 meters for the division of the home fire emissions, because in "scale" analysis we define as "scale" half the wavelength of a spatial variation. Through the 9 grid points we can resolve a square with a side length of 1 kilometer.

To be sure, the meteorological conditions alone do not determine the spatial "scale" for home fire emissions. There is also the structure of the built-up area density. For central European cities, the "scale" derived from the spatial structure usually agrees well with that given above. At least, this applies for cities with horizontal dimensions from some 10 x 10 km up to 25 x 25 km. For smaller ones, it may be necessary to

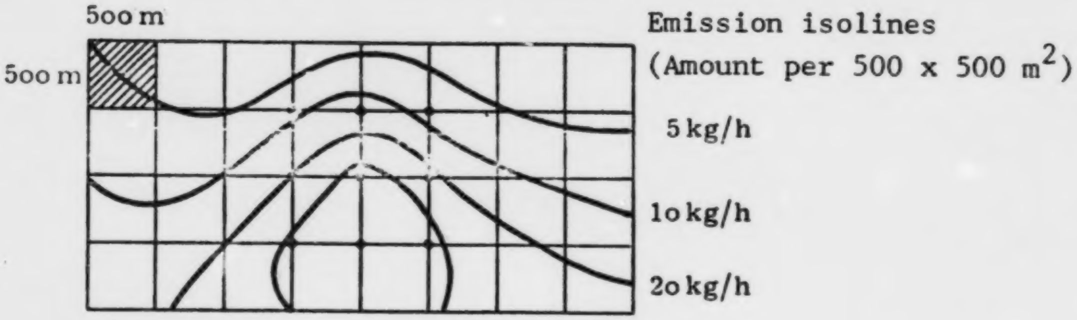

Figure 6. On the concept of the "scale" of the spatial variation of home fire emission.

choose a smaller area size, and perhaps a larger one for larger cities.

Figure 6 represents a home fire emission field spatially averaged in the "scale" of one kilometer. All finer differences are averaged out. This field of home fire emission can now be represented as a spatial function of the type $Q = Q(x, y, h(x,y))$. The source strength at a point x, y of the field depends on the local emission, and is also associated with a local emission height $h(x, y)$. The local emission height h varies considerably within a city, for instance, between the suburbs and the city center. It also depends on the meteorological parameters, which enter not only into the smokestack superelevation but also into the special flow conditions in the vicinity of a house.

It is understandable that one will never be in a position to consider exactly the variability of the local effective stack heights on one hand, and the exact isoline arrangement of the emission according to Figure 6 on the other hand. Further approximations are necessary and reasonable for modeling purposes. First, we take the average of the emission for each area element and plot it in the element as a number. Figure 7 gives an example

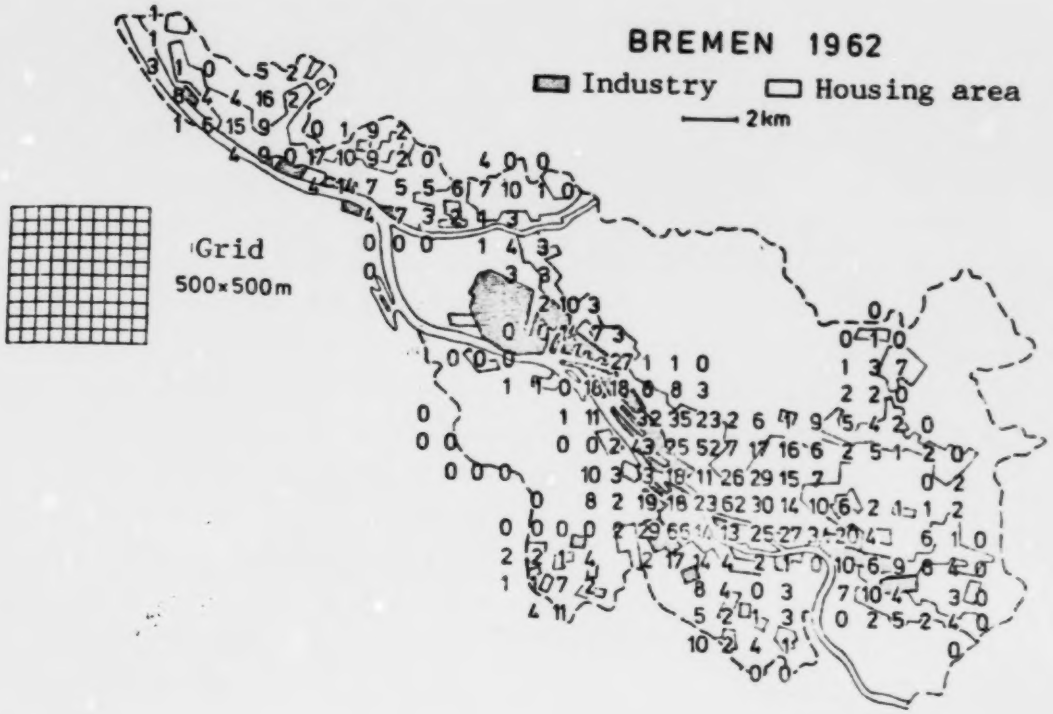

Figure 7. Emission register of home fires for Bremen. The values indicate kg SO_2 per square kilometer.

of this process for the city of Bremen. There, for a simpler presentation, the total emissions are given for area elements of the magnitude of 1 x 1 km. In addition, we assume a uniform effective emission height h for each area element. A change of this height from area element to area element is not easy to consider, however, or to observe clearly within a city.

It is often emphasized that home fire emission is equivalent to emission from an area source. This statement, however, is correct (in the sense of a very good approximation) only for the case in which the spatial dimensions of the region are very large in comparison to the separations between the actual home fire sources. Then, in a "scale" with the dimensions of a large congested area, we can assume that the superimposition of the smoke plumes which are close beside each other is so complete that the effect of discrete sources will no longer be detectable. The result then is the same as would come from assuming an area source. We can see that even here the "scale" concept plays a decisive part. In the study of the immission conditions for a smaller neighborhood, the requirements of the statements from the immission condition modeling will be so detailed that we can certainly not work with area averages of the emission and with area sources. As a marginal comment, turbulent diffusion also produces a characteristic "scale" and there are great differences in the approximations determined from the "scale" analysis, depending on what stability class has developed. All of this shows clearly that we must have greater meteorological as well as modeling experience before we can model the immission conditions of a region successfully.

The division of home fire emissions into area emissions of the type described has generally been accepted; but, the sizes of the areas differ (those of other authors are all larger than 500 x 500 meters, even if this cannot be justified by "scale" considerations) and there are also considerable differences in treatment of the transmission process when we are dealing with an input from an area source. In the case of the city of Bremen, it seemed to the author that it would be suitable to keep the concept of individual point sources even for home fires. In nature, these occur with separations of some 50 meters. Then each area element of the size 500 x 500 meters has 100 individual sources. In the existing concept, these are considered as completely identical. They all have the same source strength within the area element, and the same effective emission height. The sum of the 100 source strengths yields the average total emission for the area element. A typical value from Figure 7 is 20 kg/km^{2}hr = 5 kg/(500 m)^{2}hr. Each individual chimney, then, emits 50 g/hr on the average, representing some 5 to 6 dwelling units. Because the spatial separation of the sources from home fires is still maintained, the superimposition of the smoke plumes in the vicinity of the area element or inside it is not quite as complete as for an area source; but, at a distance where the maximum immissions generated by the source appear,

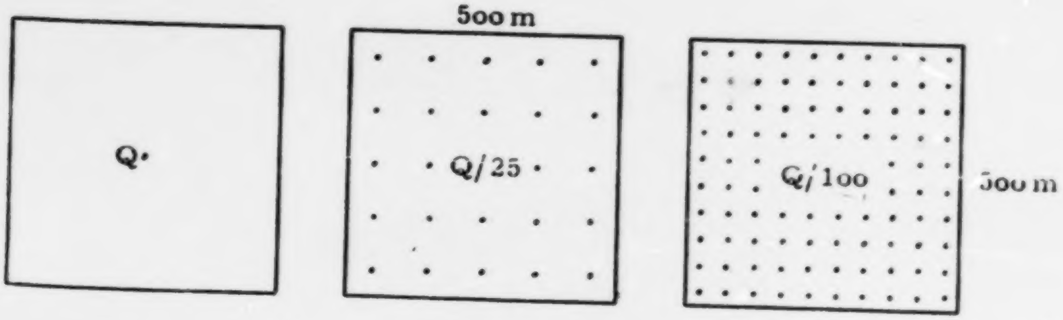

Figure 8. Representation of area emissions by a multitude of individual point sources.

this superimposition is so complete, for 100 sources per 500 x 500 meters, that the immissions no longer differ from those of an area source.

In this relation, we must remember that the turbulent propagation conditions (characterized essentially by the standard deviations σ_y and σ_z) determine the extent to which the superimposition process is completed for the individual smoke plumes. For unstable layering, this leads rapidly to complete superimposition, but only to relatively incomplete superimposition for stable layering. For a separation of 50 m between the individual point sources (100 sources per area unit of

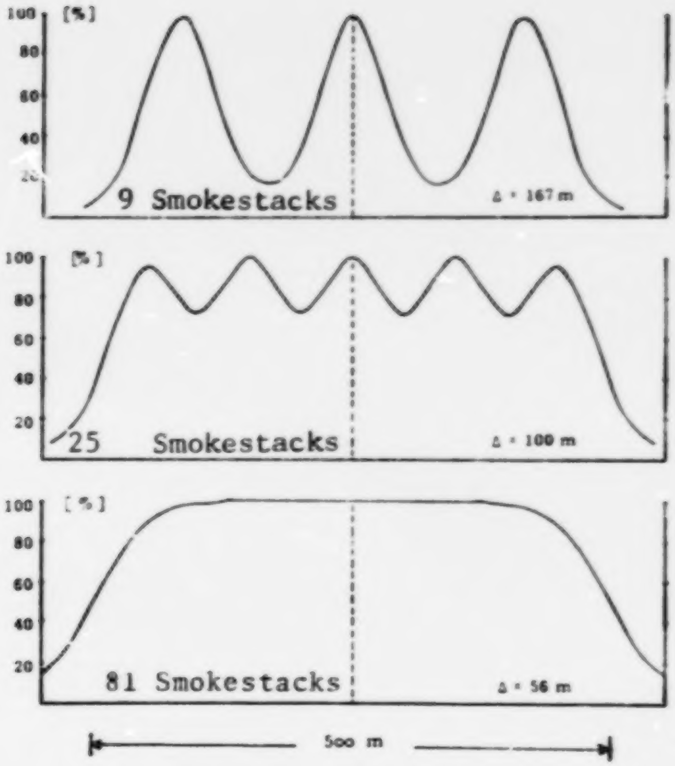

Figure 9. Concentration distribution, transverse to the wind direction, in the lee of an area source, represented by an increasing number of point sources.

500 x 500 m), however, the superimposition is adequate under all stability conditions. Figure 9 shows an example.

Simulation models for an immission climatology differ, among other things, in their treatment of house fire emission. This difference is always greatly emphasized, although there are differences in the scientific establishment of objectives which decide the true value, or lack of value, in such a model. The model for Bremen is always named as an example for a model which simulates area sources by a large number of individual sources in a very expensive manner. It is generally not particularly considered that it is the first and only model for a complete immission climatology of a region with high information output. We see from this how important the source representation is still considered, and that we are not urged on to more extensive problems. There is agreement, among other things, that a so-called true area representation is to be preferred to all approximate representations. In fact, it is also possible to set up a steady point source arrangement and to state the resulting immission distribution in the form of an integral through integration over the area element. Unfortunately, though, there is no analytical solution for the integral, due to various mathematical circumstances, and we are forced to a numerical solution. But this numerical solution has exactly the character of a representation using many sources, and we come back to this method. Such experiments were done [25] with the result that the representation using many sources, with a far smaller number than our 100 sources per 500 x 500 m, was adequate to describe the immission distribution in the lee of an area element. But the studies in [25] also showed that an often-used method of representing an area source using a line source at the windward edge of the area source is scarcely suitable for use in simulation modeling. This is true to a much higher degree for the representation of an area source with a single point source at a certain distance from the upwind edge of the area source. The poor simulation results often reported by American authors are due to this type of area source representation.

For the case of large congested areas, the lateral turbulent diffusion (expressed by the standard deviation σ_y) plays a part which is smaller the larger the region is. Then the propagation theory considers only the turbulent diffusion in the vertical direction and, of course, the spatially variable wind field. Here, under certain circumstances, it is even possible to give analytical solutions for area sources, using constant vertical diffusion coefficients. Such investigations [26, 27] served as guidelines in the development of the Bremen model.

If we keep in mind the process of emission determination for house fires, as was depicted before, then we see that as a result of using area averages and of representing the emission by many identical point sources in a regular arrangement, it appears that we need only an estimate of the emission register for house fires. It would probably not be worth the cost to spend too much in collecting house fire emissions if we plan to simulate an immission climatology. The situation might be different for the purpose of temporal immission predictions. There, higher accuracy is needed, even in the spatial resolution of the immission fields, and this reacts on the accuracy requirements for the emission register. Only accurate "scale" analyses of the type indicated earlier would be able to make binding statements about the requirements for the emission field. At present, to be sure, such analyses do not exist. Only the modeling experiences of a certain group of authors are available. Even today, though, they form the basis for expensive emission collections in many countries of the earth. Such collections are being undertaken most extensively today in the United States, where it is one of the obvious duties of the air pollution control offices of the cities to establish emission registers. In the background there is the goal of a mathematical-meteorological simulation of the immission conditions to work out control and planning strategies. Similar efforts are also under way in many European countries and in Japan.

We have previously discussed the assumptions which have been used with respect to the emission register for the simulation of the immission climatology. In comparison with other congested areas, the emission collection for the Bremen region was done relatively easily. But other conditions, too, made Bremen seem particularly suitable for the first numerical experiment. The other input data for the model were also relatively simple. Distant sources which could generate background immission could play a subordinate part in the case of Bremen. The nearest large cities (Hamburg, Hannover) are some 100 km away and smaller cities (Bremerhaven, Wilhelmshaven, Oldenburg) are 50 km away. Except for stable weather conditions with winds from the northeast or southeast, which occur relatively seldom on a statistical average, background immission could be ignored. Special regional data also hardly needed consideration. The terrain of the city is flat enough (except for the north portion) so that we could expect the low-level wind field not to be modified by topographic effects. The other meteorological conditions in Bremen are also very favorable to modeling. As a city near the coast, it is well ventilated throughout the year. Stagnating weather conditions with inversions occur relatively rarely. Thus, many conditions necessary for modeling with a simple model were fulfilled. In spite of this, there were and are many problems related to selection of the meteorological parameters. This was discussed extensively in Chapter 2. The choice of the stability classes, the assignment of the standard deviations σ_y and σ_z to them, the class distributions of the wind strengths and wind direction, and finally the selection of a representative meteorological station are problems which must be solved in any modeling of the immission climatology for a region.

The only meteorological station with hourly meteorological observations which came into consideration was that of the Bremen airport. The wind directions measured there are an average over a certain time interval during the observation, and they are only reported as rounded off to a full 10 degrees. Some difficult

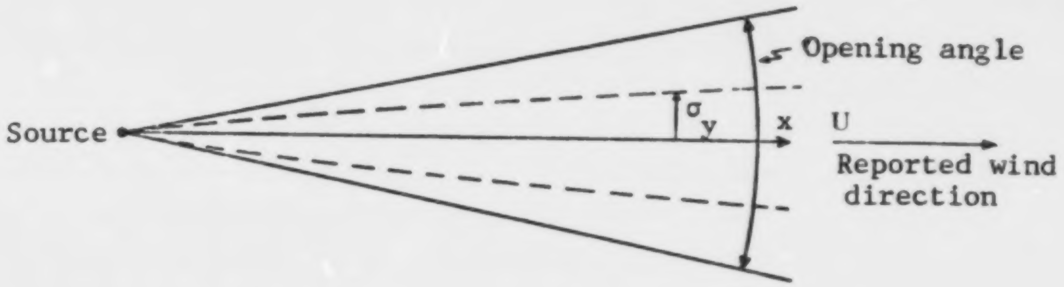
Opening angle
Source
σ_y
x
U
Reported wind direction

Figure 10. Sketch for Figure 11.

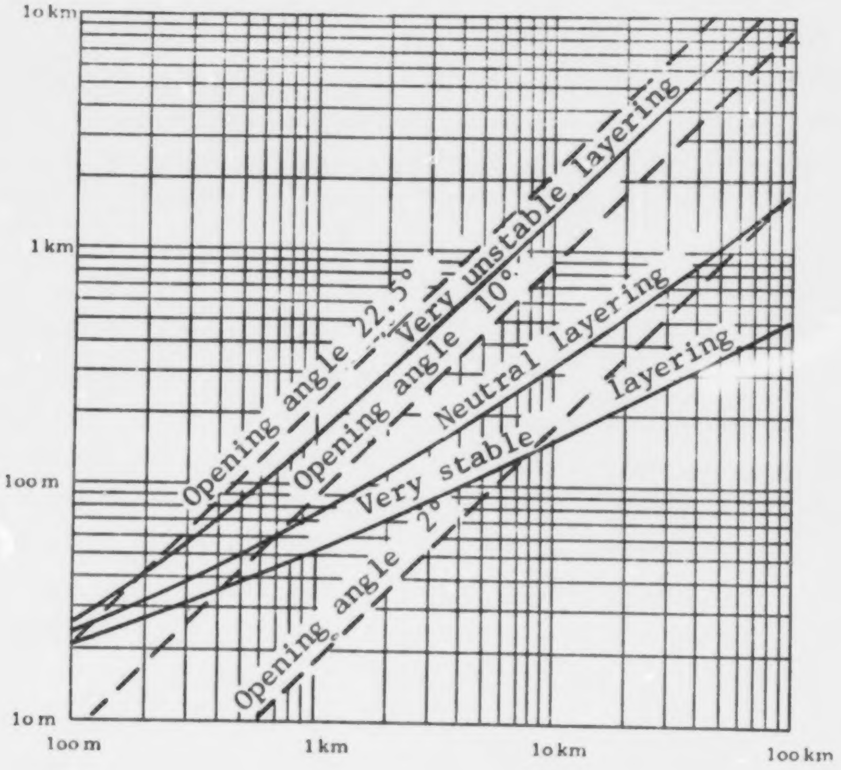

Figure 11. Wind direction sectors for various opening angles and standard deviations σ_y for two extreme stability classes (very unstable, very stable (inversion)) and for neutral conditions.

modeling problems are tied up with this. In the theory of turbulent diffusion it is shown that the concentration in planes perpendicular to the axis of the smoke plume (wind direction) can be represented by a two-dimensional Gaussian distribution with the dispersions σ_y and σ_z. The lateral dispersion σ_y gives the distance at which the concentration on the smoke plume axis for the same source distance perpendicular to the axis has decayed to the value exp (-0.5) = 0.607. At a distance $y = 2\sigma_y$ perpendicular to the axis we find only a portion which is exp (-2) or the 0.135-th part of the axial concentration. For small values of σ_y this means that the smoke plume will be closely gathered together, and for large values it means a strong lateral dispersion. Because the wind direction report is rounded off to 10 degrees, the direction of the smoke plume axis is indeterminate to ± 5 degrees. Figure 11 shows how the lateral dispersions σ_y behave for the most different stability conditions as a function of the source distances. At the same time, the left side of the angle is also stated as a function of the source distance for the opening angle of the wind direction report. If, for instance, we assume an opening angle of 10°, then we have the following for very stable layering: For small source distances of less than 400 m the lateral dispersion is so strong that the angle with the 10° opening shows no large lateral concentration difference. Inaccuracies in the wind direction report have no serious effect. The situation is different at a distance of 10 km. The "width" of the smoke plume ($2\sigma_y$) is somewhat more than 300 m, but the width of the wind direction sector at the same distance is 1,800 meters. Thus, it requires a very accurate wind direction report in order to be able to find the smoke plume in the wind direction sector. If we are dealing with a very low source (house fire), then the maximum ground immissions occur near the source (usually closer than 400 m) and we need not be concerned with the uncertainty in the wind direction report. For this type of source, this is true to an even higher degree for the other stability classes, because they show a significantly greater lateral dispersion. For large emitters, with which the maximum ground immissions are found on the order of 10 km from the source, inaccuracy in the wind direction report becomes unimportant only in very unstable layering. In the great majority of weather situations, we do not find the smoke plumes in the direction given as a rounded value. The situation is even worse if wind directions are reported according to the 16-part wind direction scale (N, NNE, NE, E) because here the opening angle is 22.5°. According to Figure 11, then, the smoke plume will not, or only rarely, be found in the reported direction even with very unstable layering and low source heights. According to Figure 11, a wind direction report with ± 1° accuracy would be good enough to suppress the uncertainty in calculation of the ground immission field, resulting from the uncertainty in the wind direction report, to an acceptable amount under all conditions. This would then apply for individual industrial sources. For house fires it has already been established that directional report accuracy to ± 5° is sufficient. From this example we see that we can find few general rules. A general conversion of all the computations to 2° wind direction intervals cannot be done because of the computing time, quite aside from the fact that the exact wind directions are not available. For those cases in which we must work with small opening angles, though, there remains no alternative other than to disperse the smoke plume not only in the reported wind direction, but also in the four adjacent directions which differ from the reported direction by ± 2° and ± 4°. Each of the five wind directions is equally probable and must be charged with a fifth of the source strength. This method was discussed many years ago in the VDI committee, "Theory of Propagation", and has also been used in verification of the Bremen model on the basis of measurements.

In modeling work, one must be very closely concerned with the problem of the representative meteorological station for a city or a region. Directional changes occur in the low-level wind field because of changes in the surface roughness. Thus, for instance, one cannot expect that the wind direction report from an airport is representative for the city region if the airport is upwind of the city due to the weather situation. These cases occur relatively often in Bremen. But it is known for other cities, too (e. g., Frankfurt) that the wind observations at the airport cannot be considered unconditionally representative for the city, so that they cannot be considered representative for the model computation. Special meteorological investigations will make up the most important part of the work in every region to be modeled. This is particularly true for the understanding and statistics of inversion weather conditions which have been discussed earlier. The model developed for Bremen is able to include the blocking effect of an inversion fully in calculation of the ground immission fields. No other model can do this in the same way. Unfortunately, no use could be made of this model capability in Bremen because we could only rarely (hardly more than 5% of the days in 1962) establish inversion weather conditions with low inversion heights (250 to 300 m) from the radiosonde ascents of the radiosonde stations, most of which are 100 or more kilometers away. Routine radiosonde ascents give no answer about the presence of even lower inversions. The effect of these on the immission situation was depicted earlier. More accurate investigations were begun with the Bremen model. Figure 12 shows the result of an inversion experiment. With the aid of the complete model equations, and using the emission register for house fires and industry, the ground-level immissions generated by industry and house fires were calculated separately for one location within the city and for a definite meteorological situation. The location was selected so that the immissions from both source groups varied within the same order of magnitude under those weather conditions. This was about 0.2 mg SO_2/m^3 for each source group in the absence of inversion. Then an inversion was included, and its height was reduced in steps from large values. For house fires, for which an effective emission height of 25 m was used, the ground immission generated was practically unchanged down to an inversion height of 100 to 150 m. Only with inversion heights below 80 m was there a rapid rise in the ground immissions with continued decrease in the inversion height. For an inversion height of about 40 m, the immission had already doubled over the starting point; and it had quadrupled for a height of just above 25 m (emission height).

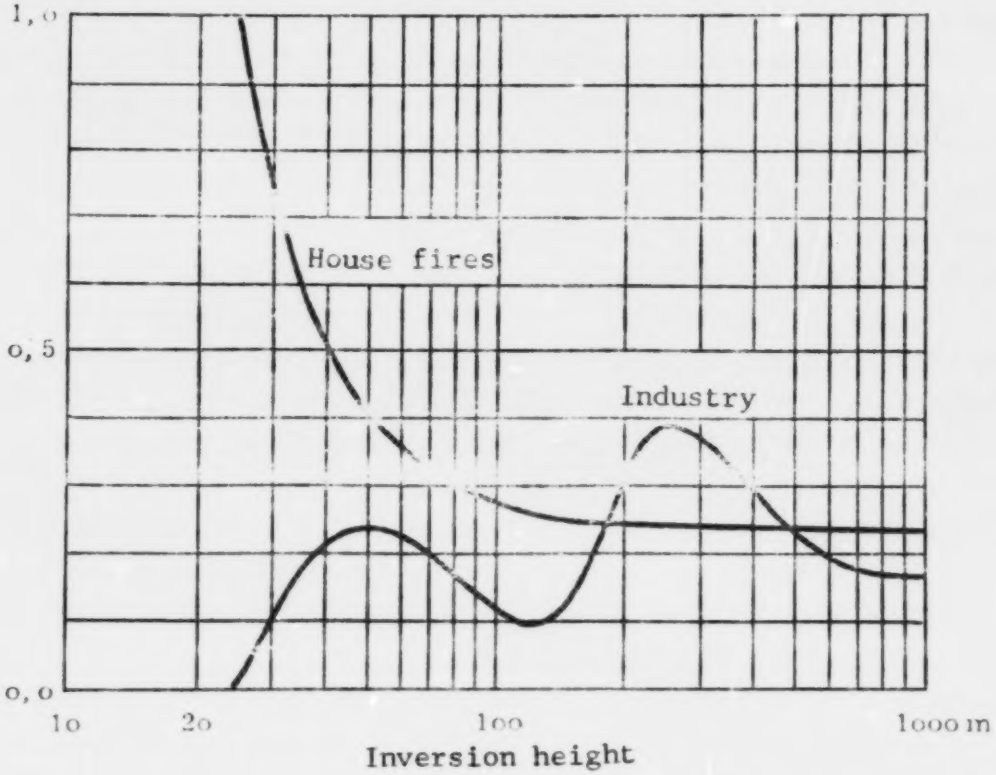

Figure 12. Ground immissions (mg SO_2/m^3) as a function of the height of an inversion for a location in Bremen and for a definite weather situation, for house fires and industry separately.

A complex picture appears for the industrial situation (highly varying emission heights). It has long been known [28] that the maximum ground immission generated by a point source depends very little on the height of an inversion which makes an upper boundary of the spreading volume if this height is more than twice the effective stack opening. As the inversion is forced down to just above the effective opening, the maximum ground immission rises to double its value in comparison with the inversion-free case. Also, ground immissions which are all higher than in the case of absence of inversion, occur in a large region. Because an inversion, being a stable layer of the atmosphere, strongly damps the thermal buoyance of the hot waste gases, the stack superelevations are reduced as the inversion is lowered, until the hot waste gases break through the inversion layer or until the stack opening is above the inversion. The process of reduction of the stack superelevation as the inversion lowers is difficult to comprehend numerically; only empirical trial solutions are available. The importance of this effect is unusually great, however. Stated crudely, the maximum ground immission is inversely proportional to the effective stack height. A reduction of the effective height becomes apparent in an increase of the ground immission, and the more so the lower it is. There is also the rise which has been mentioned as a result of the blocking action of the inversion.

In the city, we must be greatly concerned with the frequency distribution of the effective smokestack heights of the industries if we wish to investigate the effect of a sinking inversion on the ground immission. According to Figure 12, there appear to be two principal groups of large emitters in Bremen. One group has (reduced) effective stack heights of about 250 m, and the other has stack heights about 50 m. If the inversion sinks to heights below 600 m, then an increase in the ground immission occurs at the location where the inversion is in the vicinity of the first stack with an effective stack height of perhaps 300 m. On continued sinking, more and more new emitters come into the range of the inversion, generate high ground immissions, and separate from the register as soon as their openings are above the inversion. At an inversion height of some 125 meters, a whole group of emitters has separated from the emission register in this way, but the inversion has not yet reached the height of the effective stack heights of the next emitter group. This occurs at 80 to 50 meters with further sinking, so that this group generates its maximum ground immission values due to the existence of the inversion. As the register contains no industrial chimneys with effective stack heights below 25 feet, the industrial emission no longer contributes to the ground immission for very low inversion positions. The ground immission is then generated solely by house fires.

The experiment described above was performed, as an example, for only one location and for only one meteorological situation (wind direction, wind strength, stability class) in order to show in what a complex manner the ground immissions build up under the influence of a blocking inversion. But the experiment also shows what possibilities there are for a control strategy if one has such a model. If one performs such computations for each location (at a distance of 500 m from each other, or selected arbitrarily) within the city region and for every meteorological situation, with the inversion altitude being included as a parameter along with the other parameters which are important for propagation, then one can make the following statement, for example, for the location to which Figure 12 applies: At a predicted inversion height of 250 m, the source group of highest emitters must reduce their immissions by 50% in order for the ground immission, as the sum of house fire immission and industry immission, to remain below the value of 0.5 mg SO_2/m^3 at the location under consideration. All the smaller emitters are not affected by the control measured. At a predicted inversion height of 125 m there are no control measures at all. The sum of the ground immissions generated by house fires and small industry is below the prescribed value of 0.5 mg SO_2/m^3. The group of large emitters emits into the space above the inversion, and is subject to no emission limitations because the waste gases emitted there do not reach the ground. If an inversion height of 50 m is predicted, then the small industries alone must drastically limit their emissions, because house fires now become the major cause for high immissions. For inversion heights below 40 m the whole industry can emit again, but house fires must now be limited.

From this example we can see particularly clearly what a responsible and difficult problem it is to work out, apply, and defend control strategies. It can certainly also be seen that results of the type shown in Figure 12 can be obtained only with the aid of a mathematical-meteorological model.

The emission register for the region under consideration provides the basis for all statistical investigations in the field of air quality maintenance. On the basis of the emission register, a matching immission field appears for every classifiable meteorological situation (wind direction, wind strength, propagation conditions) in cooperation with any topographic factors. This is computed at the points of a grid net laid over the city or the region. Because of the usually more or less homogeneous meteorological conditions, it is reasonable to choose the "scale" of the emission field as that of the immission field; that is, a grid point separation of 500 m. Then, in a city of medium size (5 x 5 km^2) there will be at least 121 grid points; in a larger city (10 x 10 km^2) at least 441 grid points; and in major cities (20 x 20 km^2) at least 1,681 grid points. In general, we can figure on about 2,000 grid points for which the immission values must be determined.

The number of meteorological situations depends on the fineness of the class division of the meteorological parameters and on the class division of the additional parameters (of topographic nature, for instance). From what has been said before, division of the wind directions into 36 classes is allowable only for house fires. For individual sources, we cannot avoid using 180 classes. The wind strengths are divided into classes with regard for the character of the turbulent propagation so that on transition to an adjacent wind strength class the change of the ground immission takes on similar values over the whole wind strength range; that is, so that no irregular jumps in the immission are generated by the class division. This condition is fulfilled to some extent if we divide $U^{\frac{1}{2}}$ into classes linearly. This corresponds to the series for $U^{\frac{1}{2}} = 1.0, 1.5, 2.0, 2.5, 3.0, 3.5, 4.0, 4.5$, and the wind velocity series $U = 1.0, 2.25, 4.0, 6.25, 9.0, 12.25, 16.0, 20.25$, with U in meters/second. If we combine all the wind velocities above 20.25 m/sec into another class, we obtain 9 wind strength classes. To this we add 6 classes to characterize the turbulent propagation conditions and a large number of classes for the heights of inversions. This number depends on the local factors, and particularly on the height distribution of the effective stack heights. From Figure 12, one would choose for Bremen the class division of inversion heights of the type $H_I = 25, 35, 50, 75, 120, 175, 250, 300, 400$, greater than 400. This makes 10 classes. The height is given in meters. When we use a 36-part wind rose, this gives theoretically a total of $36 \cdot 9 \cdot 6 \cdot 10 = 19{,}440$ combinations of parameters. There are 97,200 such parameters when we use a 180-part wind rose. In the most unfavorable case, that is, when we consider topographic effects, it can be calculated that one immission field must be simulated by the model for each of about 100,000 different transmission situations. In their totality these fields make up the immission register. Expressed in numbers, this means that for 2,000 grid points the immission register can consist of something on the order of 200 million numbers. This immission register represents the totality of the immissions possible in the area, according to the emission register. When the emission register changes, then the immission register changes simultaneously. Both must always be kept current for the purpose of immission-climatological investigations. Only very large and very fast electronic computers are able to do this. Figure 13 gives one example for an immission field from the Bremen immission register.

Now let us turn to those problems in the area of air quality maintenance which can be solved with an immission register based on an emission register. These, in the simplest case, are investigations for single points within (or outside) the city. They can concern, for instance, the location of an air quality monitoring station, or the location for which a hospital is planned. If one uses climatological transmission parameters, then one can produce various types of statistics for any given time period (winter, summer . . .) from the values of the immission register at this point. One example is the calculation of the immission wind rose. Here one holds the wind direction constant and calculates, from the frequency distribution of the other meteorological parameters, using the immission register for this point, the immission occurring. If one does this for all wind directions considered necessary to represent the fields, then one gets a view of how often, and from where, the point is loaded with immissions. If one is interested in the average load from the various directions, then one takes the average from the individual frequency distributions and plots it in the direction from which the corresponding wind comes. This gives the immission wind rose of the averages. Figure 14 gives an example from Bremen. But this does not exhaust the information

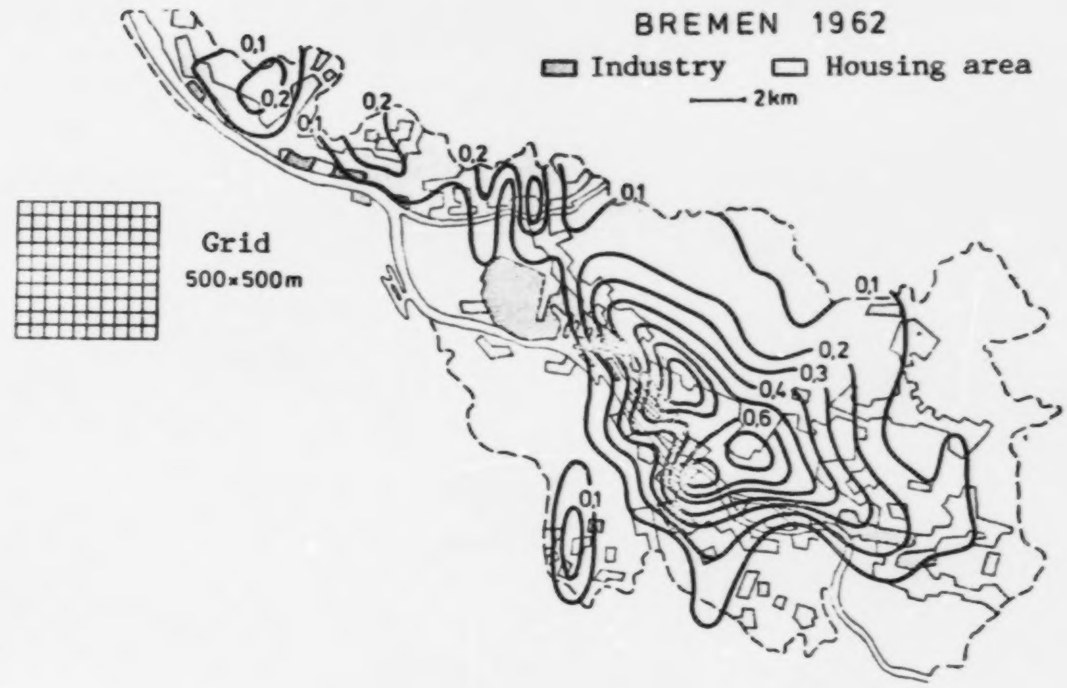

Figure 13. One specific immission field from the immission register (for a certain combination of meteorological parameters).

content of the calculated frequency distributions. One could, for instance, align the relative frequencies for each class (in percent) beside each other for each direction, then, by connecting the endpoints for each class, obtain a very clear picture of the direction-dependent frequency distribution. Figure 15 shows this schematically.

Representations of the direction-dependent frequency distributions of the nature of Figure 14 have the highest information value for planning purposes. If one procures these data for each grid point of a region, and for all the time periods of interest, then one perhaps has the most complete

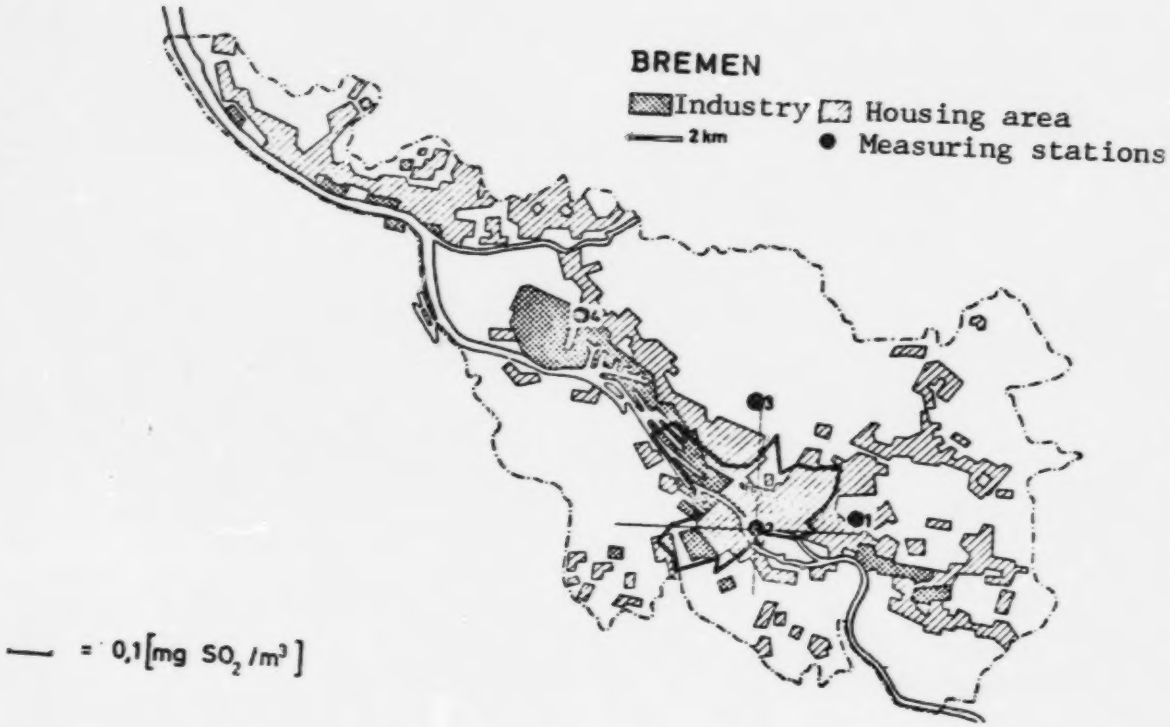

Figure 14. SO_2 wind rose at Station 2 for the heating period.

picture which can be obtained from model simulation. The highest requirements are placed on the quality of an immission climatology model if it is desired to simulate the isolines of the presentation of Figure 14 at each grid point with a prescribed small percentage deviation. The requirements are less if it is only desired that the frequency distributions be simulated at each point, without considering the direction, with low error. The least requirements are made if one attempts merely to simulate a yearly average for each grid point. This is the goal of most foreign modeling attempts. The Bremen model aimed from the beginning for the simulation of direction-dependent frequency distributions, even though only calculated and measured frequency distributions were compared in the verification

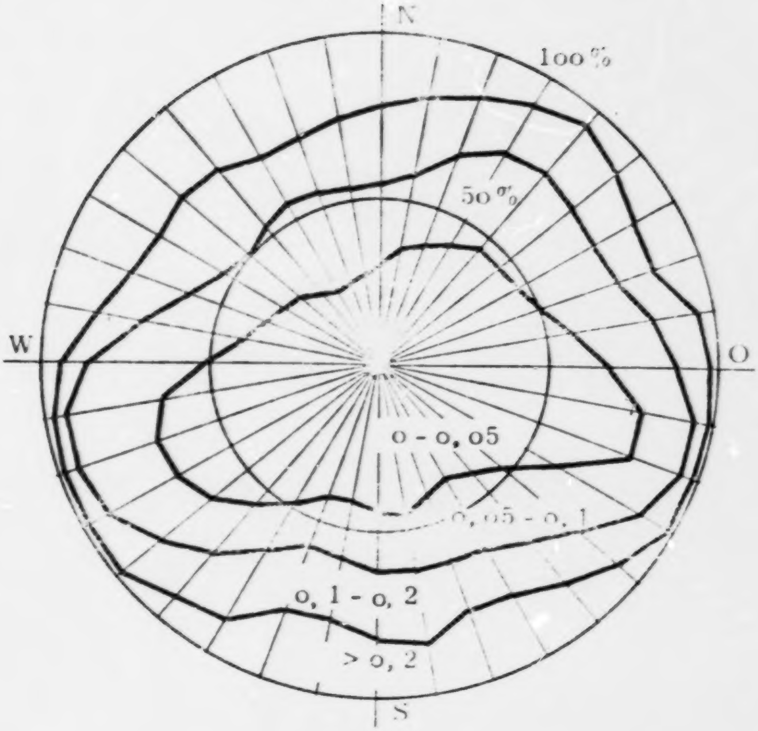

Figure 15. Hypothetical wind rose of the immission frequency integrals. Class division in the dimension of mg/m^3.

of the model through the measuring program, without considering the direction. This comparison is shown in a later figure. One reason for aiming at simulation of the direction-dependent frequency distributions is that one very rapidly gets a survey of the nature and magnitude of the load at a location as it depends on the wind direction. Another reason is that it must be possible, using these presentations, to indicate solutions for the problem of determining the main sources of the load.

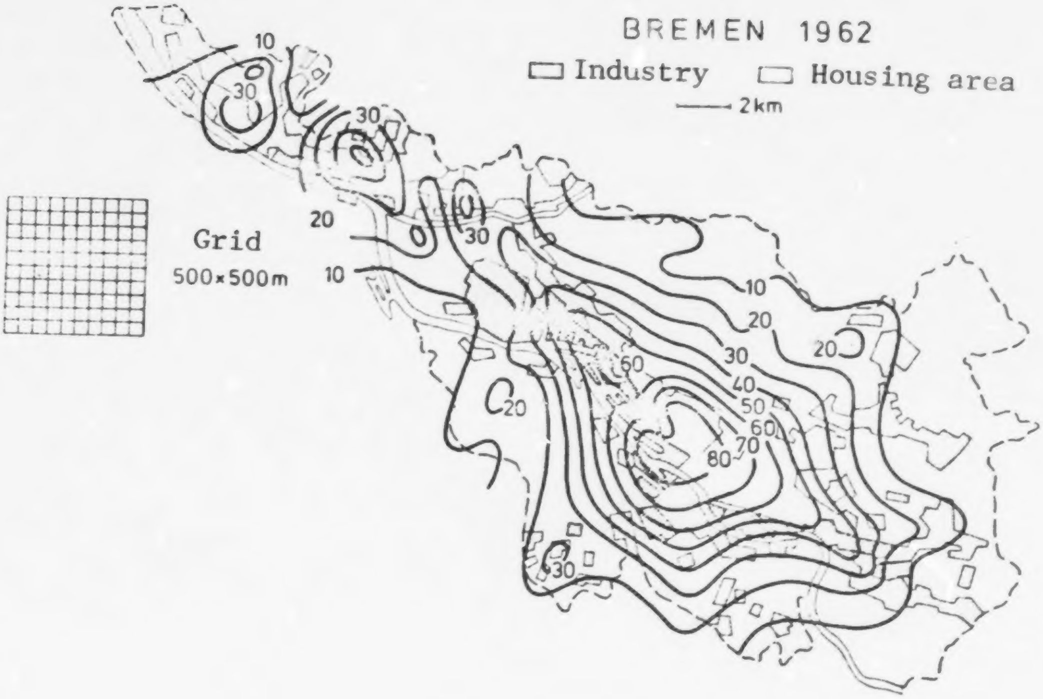
BREMEN 1962
Industry
Housing area
2km
Grid
500×500m
10
30
30
20
10
30
10
20
30
20
60
40
50
60
70
80
20
30

Figure 16. Percentage of the hours in the heating period with immissions greater than 0.1 mg/m^3.

For city planning purposes, the immission frequency distributions arranged according to the wind direction are not sufficient. As indicated previously, one determines the characteristic statistical quantities of the frequency distributions and represents them on a map. Figures 16 and 17 show two such parameters, presented on a map, for Bremen.

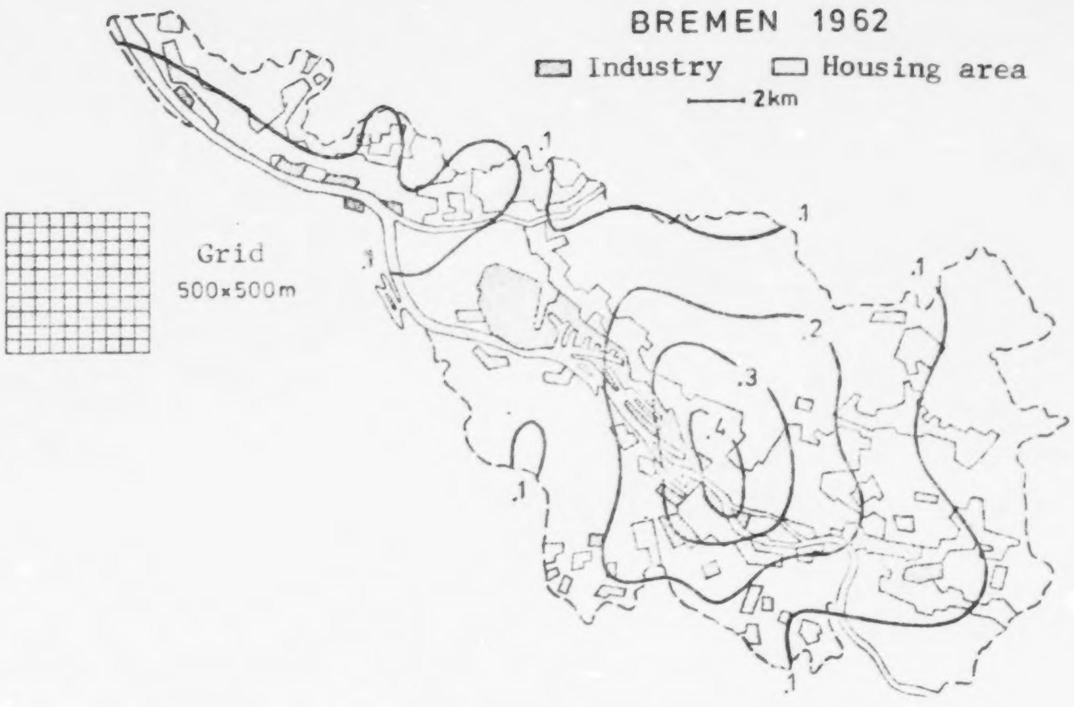

Figure 17. 97.5% confidence limits.

Figure 16 shows the percentage of the hours during a heating period in which the ground concentration of SO_2 exceeds the prescribed value of 0.1 mg/m^3, as a function of the location within the city. The value of 0.1, interpreted as a half-hour average, represents a very small value and is characteristic of rather unloaded air. The figure shows that fewer than 20% of the hours of the heating period show "clean" air in the center of the city. The outer districts (except for the northern parts of the city) show pure air in more than 80% of the hours of the heating period. This parameter certainly has a high planning value. In any case it is higher than that of the average, which with a value of 0.15 mg/m^3 in the city center and a flat spatial curve shows few characteristic features. Figure 17 shows another important parameter. This is the so-called 97.5% confidence limit. The isoline in the city center with the value 0.4 indicates that for locations on this line, only 2.5% of all the hours of the heating period showed concentration values which were higher than the reported value. This parameter, which states a limit on the side of high immissions, likewise has great importance for establishment of criteria for city planning problems. It can still be mentioned that it is also possible to calculate the well-known I_1 and I_2 values of the TI Air [1] by using the immission register.

The results above have been published in various places [3,4,5] and lectures have been presented on the present state of development at some meetings. Therefore, we shall give only some major considerations on the method and its practical applicability. First, the principles. In order to simulate an immission climatology, we simulate a register of immission fields, which arose from a classification of the transmission conditions with use of a diffusion model. The discontinuous representation of the transmission conditions allows the use of models for individual sources, which proceed from the assumption of a stationary smoke plume which can be interpreted statistically. This has the result that an actually occurring immission field, in the time course of the transmission conditions, can be different from any immission field of the immission register. Due to the inaccuracies which still exist in the establishment of the meteorological parameters it is even possible that, for meteorological conditions corresponding to those for which there is an immission field in the immission register, there can be a discrepancy between the calculated and measured immission fields. This is because a stationary immission distribution cannot be produced because of non-steady transient changes in the meteorologic parameters. Therefore, if we cannot assign high accuracy to the individually simulated immission fields, in comparison with nature, can it be possible that statistics will yield usable results with such immission fields? It has not yet been possible to answer this question theoretically. The number of influencing parameters is simply too large for investigations of this type. Thus, nothing remains but to probe and to hope that through comparison with suitable measurements from a directed measuring program we will gain the potential to relate the model to the measurements by variation of the parameters; that is, to calibrate it. We will discuss the model verification in the next chapter. Here the concept of the directed measurement already pops up. It has a close relation with the problem of strategic planning of measuring sites.

One very important area of application for model simulation of the immission climatology of a congested area is that of the strategic planning of air quality monitoring nets, which cannot be avoided even if we have a model for the region. This is because the model should be continuously certified by measurements, and because there are always transmission conditions which cannot be represented properly by any model yet developed. Next is the construction of a regular net of measuring sites, such as has been done in a preliminary way by the State Institute for Immission and Soil Utility Protection in the State of Nordrhein-Westfalia. We refer to the literature series from this institute. Unfortunately, such a measuring net is quite costly in finance and personnel. Here there could be a very cost-saving field of activity for mathematical-meteorological simulation, to the extent that a model, once correctly calibrated, must be able to interpolate mathematically between a relatively small number of measuring points. The model developed for Bremen is already capable of this. As a result of correct simulation of the spatial structure of the immission fields even before calibration, the model gives the possibility of planning measuring points rationally according to prescribed criteria. Immission climatology gives the possibility of detecting the main immission points. Also, in the determination of the statistical parameters of the frequency distributions to be expected, it gives more help for planning measuring sites. Usually one can already tell from the structure of the fields how large a number of measuring sites must be erected to cover the essential features of the immission climatology by measurements in all cases. In the area described here, a model might prove itself most easily for its economic value. The cost in money and personnel to develop a model could correspond to that for the construction and one years' maintenance of a single continuously recording measuring station.

3.3 The problem of model verification

A model for immission climatology is verified if it is able to simulate immission wind roses in the manner of Figure 15 for all important points in a populated area so that prescribed accuracy requirements are met in comparison with corresponding measured wind roses. A model for predictions in time is verified if it is able to simulate the time course of the immissions for all important points so that deviations between the calculated and measured immissions remain below given limits for the same time point.

The first problem in model verification is in determining measuring locations within the region so that an optimal certification of the model can be attained by means of the measurements made there. A test calculation with parameters which are perhaps yet uncertain will certainly not be able to furnish the immission climatology parameters correctly for all points. But we can certainly expect that the spatial differences, that is, the structure of the immission fields, will be correctly described if we use a reliable emission register. The course of the isolines in the presentations of the statistical parameters for the immission frequency distributions (see Figures 16 and 17) will be more trustworthy than the numbers which are on the isolines themselves. This has been the basic assumption (and the hope) at the beginning of the work on modeling of immission climatologies. The risk that this assumption is false was very great; but fortunately we came out with a confirmation of it.

Two principles are applied in carrying out the selection strategy for the erection of measuring sites for model verification. The measuring sites should be so arranged that they include the special structures of the field of statistical praameters and also so that they are set up as unfavorably as possible for the model. The latter requirement means that in this way we will test the effect of the model weaknesses, which are known from the beginning, on the results. Now the number of measuring sites needed for model verification depends very much on the requirements for the spatial resolution of the model calculation; that is, on the "scale" of the immission field. For example, with a "scale" corresponding to a grid point separation of 500 meters, it is relatively easy in the case of Bremen to estimate where the measurements must be made in practice. If one selects the most important parameters of the immission frequency distributions for the solution of planning problems, such as that shown in Figure 16, then one will consider the following selection strategy: 1. The extreme of the isoline distribution should be included in the measurement. From Figure 16, these are three outstanding ones in the north part of the city and one in the center. Four secondary maxima at the periphery and one in the northwest part of the center are so weak that a special measurement would not be worth doing. 2. One (or more) particularly prominent isolines should be encompassed in their structure by measurements. In the case of Figure 16, the 50% line would be of particular interest. It separates regions which, more or less often than half of all hours have concentrations above 0.1 mg/m^3. The measuring sites 1 to 4 plotted in Figure 16 approximately satisfy this requirement.

3. The gradient of the isoline distribution about the principal maximum shoud be verified by measurement. From Figure 16, two lines of measuring sites would be desirable: from the center, one in the direction of southwest to northeast and one from northwest to southeast. If we calculate the number of measuring

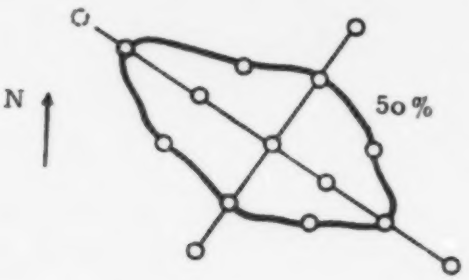

Figure 18. Desirable arrangement of measuring sites (without the northern extreme) for verification of Figure 16.

points to cover optimally the structure of the calculated field shown in Figure 16, we get: 4 for the extremes, 4 for one isoline (4 more for the isoline from the profiles), 8 for the profile, or a total of 16 measuring sites at most. These 16 measuring sites would be planned "strategically" with the aid of a model calculation. The uncertainties resulting from the still existing deficiencies of the model are vanishingly small in comparison to measuring site planning based on guesses. The economic utility of a statement that a maximum of 16 measuring sites is enough to comprehend through measurement the structure considered important is unusually great. It has already been said that the financial contribution released by saving of only one recording station would approximately suffice to develop a model.

The second viewpoint, that the measuring sites for the model should be arranged as unfavorably as possible, means the following: In the model for Bremen, the possible absorption of SO_2 at the earth's surface, the possible filtering by forest, and the effect of large water surfaces (Weser, Hafen) were not considered. Furthermore, it should be expected that an incomplete emission register would be used because of not including the emissions near the ground in the industrial areas. For these reasons, and of course for practical reasons too, because one cannot build and operate measuring sites wherever one wishes, one measuring site was installed on the Weser island near the center (surrounded by the water surfaces of the Weser and those of the waterworks) (Measuring Point 2). One measuring point was installed at the side of the Bürgerpark turned away from the center (Measuring Point 3), and one measuring site was installed in the immediate vicinity of the industry in the northern part of the city (Measuring Point 4). As only a total of four recording stations could be built, this system had to meet simultaneously all the previously stated requirements on a measuring site system. This, of course, was only incompletely the case.

The next phase in performing the model verification consists of carrying out the measuring program during a specially selected time period (this will usually be the heating period), with a meteorological measuring program needed simultaneously. The course of the transmission conditions during the selected time period will certainly not correspond with those which one has determined from processing transmission-climatological data (5 to 10 years of meteorological observations) for the time period. In the model verification, then, we can only compare actual statistical values. We lay out the meteorological measuring program so that essential meteorological model assumptions are tested with a measuring net having the density of the net of immission measuring stations. Here we deal primarily with investigations of the horizontal wind variability within the city region, and thus with the answering of questions about the spatial homogeneity of the wind fields and about the representative meteorological stations. In Bremen, recording wind measuring systems were installed for the period of the model verification (1967/68 heating period) at all four measuring sites. These wind data were compared with those obtained at the airport. Such a meteorological special program has great importance for the time of the model verification. In particular, there should be no lack of investigations on the extent of the mixing layer with the aid of vertical fine probes for the most important meteorological parameters. It has often been mentioned what a great importance the existence of inversions has for the immission modeling. In addition, intensive meteorological investigations must be linked with directed immission measurements (within the smoke plumes) during the occurrence of weather conditions with weak wind and weak exchange, so as to determine the propagation parameters valid for these conditions.

Model calculation is done in parallel with the measurement, as a time-ordered sequence of calculations of the immission fields corresponding to the weather conditions. The time course of the immission thus calculated for the immission measuring sites can be compared with the recordings. From this, we can determine whether the model developed only for climatological purposes is also adequately able to simulate the time courses of immissions. The model calculation for the purpose of model verification is relatively inexpensive, as the calculation need be done for only a small number of measuring sites. It is desirable, though, for various reasons, to set up a 500 x 500 m meter area about the measuring point and to use in this a finer computing grid with a grid point separation on the order of 125 meters. This means that we calculate the immission not only for the measuring point alone, but also for the 24 neighboring points.

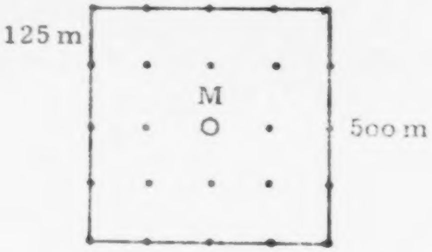

Figure 19. Grid for the model verification at a measuring site M.

In the vicinity of the measuring site we change over to a smaller "scale" and calculate the immission value at the midpoint of the grid square, i. e., at the measuring station, as a weighted average of all 25 calculated individual values. This corresponds to a suitable area averaging. If house fires were the only sources of immission, this type of area averaging could be omitted. But it is necessary to determine the load from individual sources with small smoke plumes under the nonsteady propagation conditions during the measuring period, so as to consider the load at the measuring site through the smoke plumes with varying directions. It must also be mentioned that for the individual sources it is practically necessary to figure on a 2° division of the wind direction.

After the conclusion of the measurements and calculations, only the statistical properties of the frequency distributions are compared. They must agree with each other within prescribed tolerance limits. We can see from the presentation in Figure 20 that the frequency distributions do agree, and some of the agreements are outstanding. Figure 20 shows the calculated and measured frequency distributions as well as the frequency integrals for the verification period 1967/68. In case of poor agreement at all measuring sites, suitable parameters of the model must be changed to calibrate the model so that the agreement between calculation and measurement becomes equally good at all the stations. A method called "sensitivity analysis" contributes to a decision of which parameters must be varied. Each model reacts differently to changes of its parameters. To study this systematically is one of the most important works during all the model development. In the so-called Gaussian models, of which the model developed for Bremen is one, there appears a high dependence of the results on the functional form of the standard deviation σ. The representations for σ given in the literature arise from diffusion experiments under idealized conditions. In particular, complete homogeneity is attempted with respect to the ground roughness. The parameters which determine σ change with the surface roughness. In the individual case we must find which parameter must be chosen for the region concerned. In the case of the modeling of Bremen, these parameters lay between those which were obtained on the prairie and those for major American cities. This fact, though, could already be conjectured from "scale" considerations.

In the case of poor agreement at single points and good agreement at the others, one will conjecture that the modeling of the immission conditions is inadequate for the vicinity of this point with poor agreement. In the case of Bremen, the inadequate emission register in the industrial area, where only

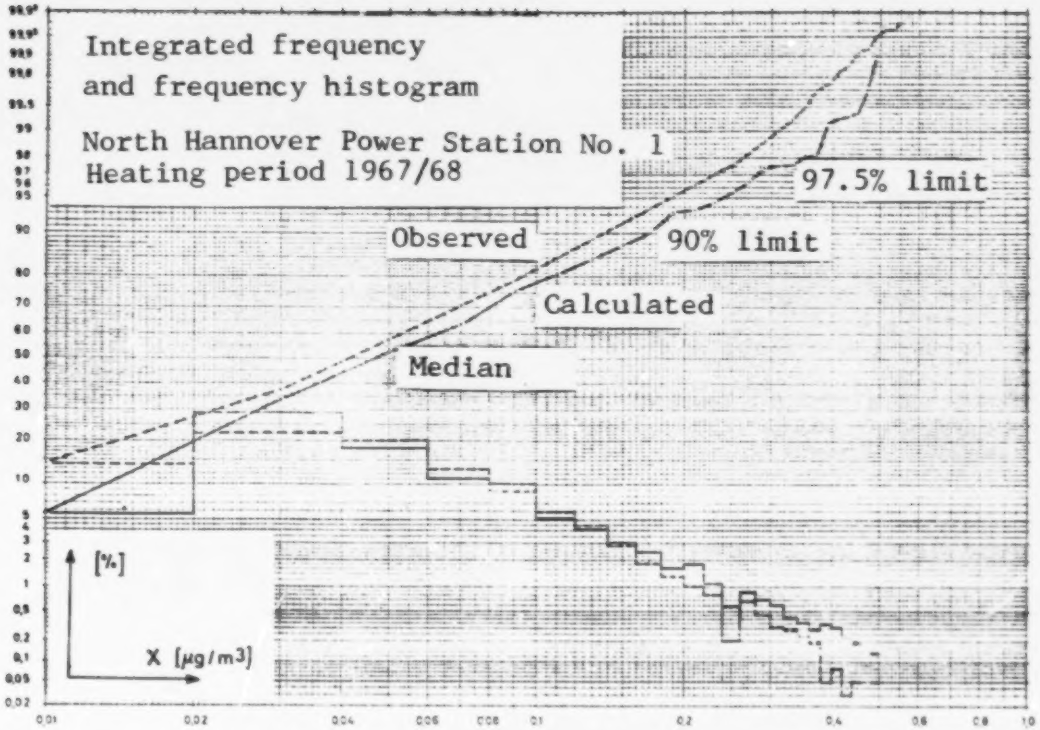

Figure 20. Comparison of calculated and measured frequency distributions (Measuring Point 1).

high emitters were registered, became immediately apparent in an inadequate description of the frequency distribution at an adjacent station (Measuring Point 4). Here the model systematically underestimated the immissions. But in this case it is not difficult to include the low area sources within the industrial region in the emission register so as to get optimal agreement between measurement and calculation for this station also. At Measuring Point 3, the model overestimated the higher immission values in particular. Perhaps the concentration-reducing effect of the Bürgerpark was responsible for this. This can be considered, in the way of experimental modeling,

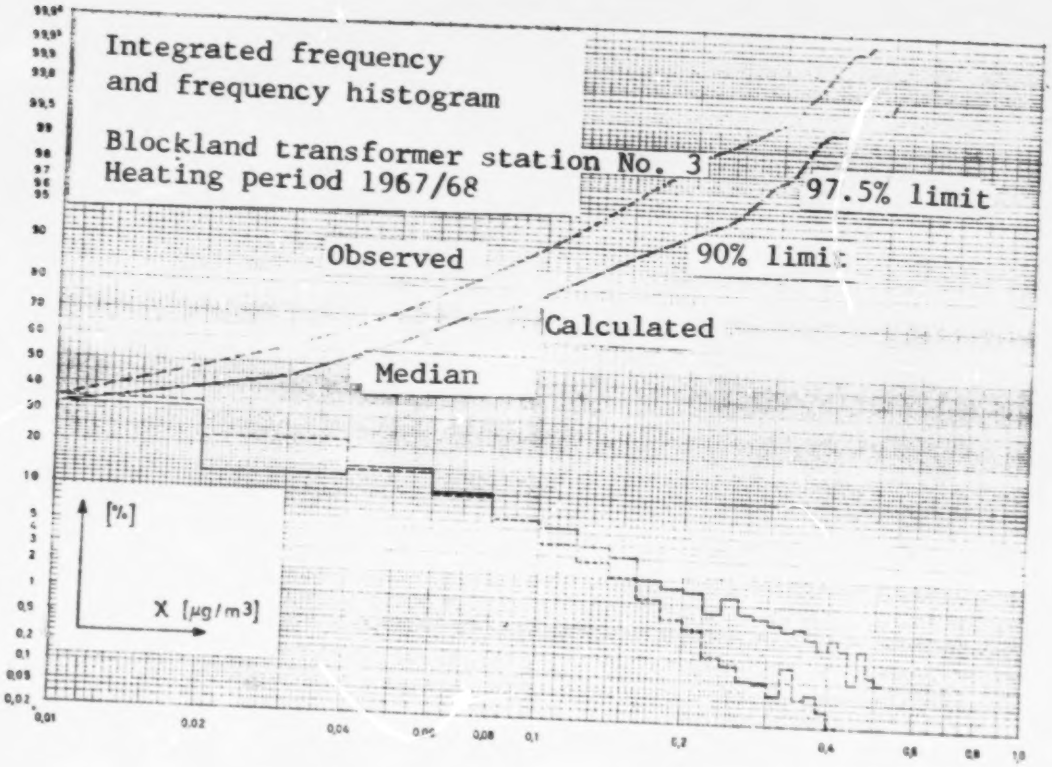

Figure 21. Comparison of calculated and measured frequency distributions (Measuring Point 3).

by appropriate negative area sources, and the method was optimated in this way here, too.

An investigation of the results from measurement and calculation at Measuring Point 1 showed that in modeling one must consider the modifying effect of large areas of water on the transmission process. In the winter, the relatively warm water of the Weser modified the air stability in the sense of destabilization. The temperature decrease with the height is then perhaps greater than would correspond to the adiabatic value of

1°C per 100 meters. This leads to stronger vertical exchange above the water surfaces and so to a reduction of the ground immissions at a greater distance from the sources.

We see that it requires relatively great effort and experience to undertake such modeling experiments. The experience is based particularly in the knowledge of the model sensitivity to changes in the parameters or in the external conditions described previously. From experience, the modeler will set many things correctly at the beginning, and can avoid further expensive experiments, most of which he has behind him. Nevertheless, new problems always remain in the modeling of a city. In the case of Bremen, for instance, the SO_2 emission of the rail traffic and of the shipping traffic was not known. This raised the problem of how one can build such temporally fluctuating linear emissions into an immission climatological model. It is questionable whether the statistics for these emissions have been established successfully so that the statistics can be associated with the transmission conditions. One has similar problems when one wishes to consider the house fire emission dependence on the time of day. There is a close relation here with the meteorological parameters, on one hand, and with the daily rhythm of human activity on the other hand. From these reasons we can expect that the frequency distributions of the immissions will change if one takes this effect into consideration. For instance, a maximum house fire emission occurs during the early morning hours during a time in which a stable layering with the possibility of low inversions is often found. Consideration of this effect as well as the effects of the air temperature and the wind on the house fire emissions were undertaken experimentally, but no improvement of the simulation results were provided.

3.4 Model extensions; time-dependent models

The extensively described model for the city of Bremen is, in its setting of goals, the most developed model in the group of the so-called "plume" models. The models in [29, 30, 31] are comparable in technology and model assumptions. Possibilities for improving this type of model were mentioned often in the first chapter. We referred particularly to consideration of weather conditions with weak wind and exchange in establishing an immission climatology for an inland city; to consideration of the ground topography, and to consideration of wind fields which show clearly detectable inhomogeneities within the region. Frankfurt, or the Untermain region, represents a particularly good example of a city in which one must consider all three effects.

The modeling of regions with complex meteorological and topographic conditions will probably be done with partial models in the following manner. It will certainly be possible to combine even the complex transmission conditions in such a region into groups classified in some way. One group, for instance, would be made up of all the weather conditions with weak wind and exchange. Another would be of those weather conditions in which a distinct effect of the topography can be established on the development of the wind system near the ground. Finally, a third would be those in which this is not the case. In the language of our "scale" diagram in Figure 3, it is a matter of determining for each large-scale weather condition (synoptic situation) the subsynoptic transmission conditions developing in the region, classifying them in dependence on the large-scale situation, and developing a subsynoptic transmission model for each class. Synoptic weather conditions again serve as ordering parameters for this classification. In the case of wind, these are not those already affected by the topography, but those at an unaffected level, perhaps high above the surface. The problem, of drawing conclusions about the development of subsynoptic wind systems from large-scale meteorological parameters, is not yet satisfactorily solved in meteorology. In all countries, people are working today on this problem of the interaction of the different "scales" of movement processes. Of course, for immission-oriented modeling, one must even today find solutions, and this is possible only empirically. If one has ideas on the relation between the large-scale and the subsynoptic meteorologic conditions, then, as before, one can use counting statistics, obtaining for each time interval of a period a statement of which model is to be used with which parameters. Here, then, just as before, an immission register is calculated from all the classified transmission conditions and on the basis of an emission register. In fact, such an undertaking is now in process for the Untermain region [32]. Considerable expense is necessary in the area of development of new models. The treatment of inhomogeneous wind fields in particular offers difficulties.

In the literature, people have attempted to treat inhomogeneous and nonsteady transmission conditions using other types of transmission models, namely, with the "puff" model [33, 34, 35]. In principle, this is able to calculate the time course of the immissions under the influence of parameters varying in time. The "plume" model arises from the "puff" model as a limiting transition for constant meteorological conditions and very long propagation times. Thus, the "puff" model is the more general, but it is more difficult to use because one cannot assign the standard deviations occurring there to the group of meteorological parameters in a similarly simple way on the basis of diffusion experiments. In spite of this, the results appear very hopeful [33, 34, 35] and may introduce a new generation of models, primarily for the prediction of temporal immission developments. In parallel with this, efforts are being made to find solutions for these time-dependent problems on the basis of the time-dependent diffusion equation. So far, no results which could be reported have appeared.

3.5 The optimization problem in the solution of control and planning objectives

Most recently, people have devoted themselves particularly to development of analytical solutions for optimal control strategies on the basis of mathematical-meteorological simulation models [36, 37] They are concerned with working out measures to improve existing conditions and control measures in planning extensions of emissions, from the viewpoint of the greatest possible fairness and minimum economic loss. This is undertaken while maintaining the secondary condition that the immission limiting values shall never be exceeded anywhere.

One is primarily interested in maintaining the limiting value for the yearly average of the immission from an air pollutant [36]. The so-called immission surface is the basis for such investigations. This is the surface developed by a single source as the result of steady emission and all the transmission conditions during the year. Finally, this is nothing else than if one were to establish an immission register for every single source on the basis of all transmission conditions, calculate the frequency distributions for each point of a grid, calculate from this the average (here, the yearly average) and produce a map representation of the yearly average for each individual source. Because of the direct proportionality of the immissions to source strength we can first act as if each source had the strength "1". For otherwise identical emission conditions (source height, parameters to determine the stack superelevation) these fields for the yearly average are completely identical. They are only mutually shifted according to the magnitude of the source location. The yearly average fields change with the emission parameters in a characteristic way. The function T_i (x, y), which allows calculation of the value of the yearly average at a location x, y due only to the influence of source i with the source strength "1", is called the "transfer" function and is determined by the properties of the model. The yearly average at a location x, y resulting from the superimposition of all sources with the source strengths Q_i is simply the sum of all the "transfer" functions multiplied by the source strengths Q_i: $\sum_{i=1}^{N} Q_i T_i (x, y) = \bar{s}$. Now it can be that this yearly average exceeds the prescribed limiting value S at some places. Then one experimentally changes the source strengths of all sources by the amount dQ_i. This leads to a change in the average by $d\bar{s} = \sum_{i=1}^{N} dQ_i T_i (x, y)$. The changes dQ_i are now determined so that the new average $\bar{s} - d\bar{s} = \sum_{i=1}^{N} (1 - dQ_i/C_i)\ Q_i T_i (x, y)$ is everywhere smaller than the limiting value S, on one hand, and on the other hand so that the costs of emission reduction are as small as possible: $\sum_{i=1}^{N} K_i (dQ_i/Q_i)$ = minimum, where K_i are the costs for emission reduction at the sources "i". There are also limitations of technical or other nature on the reductions dQ_i, and these must be considered.

The appropriate aids are available in mathematics for the solution of such optimization problems. They provide solutions which are elegant and relatively easy to handle numerically [38]. The idea in this method is that one does not compute statistical characteristics of the frequency distributions for each location with an immission register of superimposed smoke plumes; instead, one computes the frequency distribution separately and then superimposes these. This method is particularly adapted to the problem of an optimum control strategy, as the individual source strengths are visibly retained in the superimposition of the individual frequency distributions, so that they can be varied.

The fact that intensive work on such control strategies is going on in the United States shows clearly how much reliance is placed on the mathematical-meteorological models for the simulation of immission climatologies even today.

SUMMARY

First, the concept of mathematical-meteorological simulation of immissions is defined quite generally. Then it is shown how problems of immission control strategy can be solved in principle with such simulation models. Special weight is placed on the fact that the most important control measures (warning system and planning) can be optimized technically and economically by way of a control loop. Then the problem of development of such simulation models is discussed entirely openly, and it is shown that an abundance of problems, mostly meteorological ones, occur and cause difficulties in these developments; but, there are also a large number of physical, physical-chemical and mathematical problems to be solved in order to be suitable for the most important problems of immission-oriented environmental protection. These considerations are considered a stimulus to more extensive research.

In spite of the reported problems in model development, there are already today practically usable models for the immission climatology in the vicinity of a single source, for the area of a city, or for a region. A description and evaluation of these models leads, in the course of the discussion, to the result that the existing models are, with great certainty, suited for the solution of planning problems. Not only the determination of minimum smokestack heights, but even the planning of changes in the immission climatology (improvement measures, new developments of emitters) are possible already today using the existing models. In this relation, statements are made about

collection of the emission register and about the "calibration" of the model through measurements. It is also shown what problems have already been solved in the simulation of an immission climatology and what perspectives appear for the application of such models.

New developmental tendencies based on the existing models conclude the work. These are primarily tendencies toward the development of time-dependent prediction models for immission prediction, and toward development of methods which allow control and planning missions to be carried out optimally in the area of immission-oriented environmental protection.

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Chapter 8

APPLICATIONS OF AIR QUALITY MODELS BY EPA

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

Applications of Air Quality Models by EPA

by

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Environmental Protection Agency

One of the purposes of the Clean Air Act is to protect and enhance the Nation's air resources so as to promote the public health and welfare and the productive capacity of its population. The Act requires air quality standards to be established and procedures to be developed, promulgated and enforced to attain and maintain these standards. Furthermore, the Act strongly implies that the preferred procedures are those which limit rather than redistribute emissions, although this implication is currently subject to a great deal of debate.

It was soon clear to administrators of the Act, specifically the Administrator, Environmental Protection Agency, that the technical aspects of the charge to attain and maintain acceptable air quality requires three basic questions to be answered.

1. How does one characterize the air quality distribution?
2. How is the air quality distribution related to the emission distribution?
3. How may the emission distribution be altered to attain the air quality standards?

In the United States, the preferred method of characterizing the air quality distribution is by air quality monitoring. There is a problem, however. Monitoring is expensive. It requires great expenditures of manpower and resources for a variety of reasons. One of the more significant reasons is that the distribution patterns of pollutants is a function of the pollutant of concern. Rarely does the maximum concentrations of CO, for example, occur in the same areas as maximum concentrations of total suspended particulate matter. It is appealing, therefore, to have a mechanism to supplement the monitoring effort. Such a mechanism to simulate the distribution of air quality is an air quality model.

To relate the distribution of air quality to the distribution of emissions, considerable dependence is placed on the results of air quality models. But the perfect model is yet to be devised. Monitoring is required to ascertain whether the model which is applied simulates at all realistically the relationships between emissions and air quality.

To devise programs to alter the emissions quantitatively, temporally and spatially so as to attain the air quality standards, models are once again attractive devices. A model, hopefully validated in the process of relating the emission distribution to the measured air quality, is applied to test the efficacy of the control tactics proposed. Once the optimum set of tactics is selected and promulgated, air quality sampling programs are continued to monitor progress toward attaining the air quality goals and standards and to improve the precision of the model used, if necessary.

It should be clear that considerable emphasis is placed on the use of models in the nationwide effort to achieve the objectives of the Clean

Air Act. Monitoring data are particularly useful in providing information on the temporal variation of air quality. Data from models are particularly useful in providing information on the spatial distribution of air quality. Modeling and monitoring supplement each other in identifying, quantifying and suggesting solutions to air pollution problems. Both are necessary, but neither is sufficient by itself.

It may be well to define the meaning of "model" and add a bit to the philosophy expressed by the earlier speakers. A model is an intellectual construct, which represents reality, and can be manipulated to predict the consequences of various actions.[1]

The real world, the true physical world, is complex. In any modeling effort, a trade-off is always required between simplicity and accuracy. Rarely are two sources of pollutants identical; even more rarely are two sources so located that their emissions are distributed identically. A friend of mine once summed up the essence of the modeling problem this way: An accurate model cannot be simple; a simple model cannot be accurate.

It is unlikely that models will ever be available that are sufficiently precise so as to apply to the very great range of time periods for which information is needed or to rare events as well as average situations. Nevertheless, difficult questions arise each day. The questions demand that decisions be made in a very short time period. As a theologian once said, "not to decide, is to decide." So, recognizing that there are great uncertainties because the models and the input information required are less definitive than desired, there is a general consensus that models, judiciously applied, can provide useful information for making a great variety of decisions involving air pollution issues.

In the Office of Air Quality Planning and Standards, a considerable variety of models, developed and approved by the research arm of the Environmental Protection Agency, is applied to the following problems.

Nature of Application	Basic Type of Model
. State Implementation Plan Evaluation	Urban-Multi-Source (AQDM, IPP, SCIM) Rollback
. New Source Performance Standards (Power Plants, Foundaries, Incinerators)	Point Source
. Smelter Study - SIP (13 non-ferrous smelters)	Point Source (with terrain adjustment)
. Southwest Energy Study - SIP	Point Source
. Fuel Deficit (211 Coal-fired Power Plants)	Point Source
. Abatement Hearings	Point and Multi-Source
. SO_2 Control Hearings	Point and Multi-Source
. Oil-to-Coal Conversions (46 Oil-fired Power Plants)	Point Source
. Environmental Impact Statements	Point Source and Highway
. Indirect Source Design	Line Source
. Auto Emission Standards	Simple and Modified Rollback
. Cost of Implementation (Economic)	Direct Cost of Implementation; Energy Quality Model
. Air Quality Maintenance	------
. Network Design	Point and Multi-Source

A short explanatory description of several of the applications may be useful.

Under the Clean Air Act, the Administrator, EPA, promulgates national ambient air quality standards for certain pollutants. The States are responsible for adopting and submitting to the Administrator for approval a plan for implementation, maintenance and enforcement of the air quality standard within their State. The plan is called the State Implementation Plan or SIP. The time constraints to develop the SIP were short and the time available for evaluation was even shorter. Therefore, in many cases, EPA worked with the States to develop an approvable SIP. As a part of this effort several areas were modeled.

Though the procedure varied from State to State, in several instances the procedure was essentially as follows. Working with a State EPA asked, "How do you want to control your SO_2 and particulate emissions?" The State would propose a series of regulations and EPA would run a model on a portion of the State - an example region - which considered the reduction in emissions which would result if the regulations were implemented and enforced. If the test indicated that the air quality standards were unlikely to be attained, EPA suggested alternative control tactics. The State would consider the suggestions, often suggest additional tactics and through a series of negotiations develop a set of control regulations which the State could pass into law and which EPA believed could be approved. The model or its results might be applied several times during the process of developing and approving the SIP.

There are over 30 non-ferrous smelters in the United States. About half of them pose serious threats to air quality standards for sulfur oxide. To develop an approvable SIP, the concerned States had to know the degree of control that was needed. Most of the smelters are reasonably isolated; in all but a few cases no air quality data were available. Therefore, 13 of the smelters were modeled, using a point-source model which included an approximation of terrain influences. The modeling results were used, in part, to develop SIP's for the States concerned. There was and still is much negotiation on this matter, particularly as to the adequacy of the model used. Some monitors were eventually established to develop further supporting data. The models were extremely useful in helping to quantify the degree of control required of the smelters to enable the air quality standards to be attained.

When the oil embargo struck in late 1973, modeling efforts similar to those applied to the smelters were undertaken to determine which power plants might be converted from oil-to-coal with least threat to air quality standards. These modeling data are still being used to adjust the Nation's available supply of oil with least impact on air quality.

The Clean Air Act requires that carbon monoxide and hydrocarbon emissions from 1975 model year automobiles be reduced by 90 percent from model year 1970 vehicles. There is a provision for extending the date of achievement of the 90 percent control by one year after a public hearing. The hearings were held. Part of the hearing evidence was the results of modified rollback models applied to ascertain the effect of delaying the application of the 90 percent control by one year, to reassess the need for 90 percent control (although the degree of control was a part of the Nation's body of laws) and to assess the impact of applying lesser degrees of control somewhat before 1975. The results were useful in estimating the trends in air quality that might be anticipated, if some of the suggested alternatives were adopted, in estimating the number of air quality control regions where CO and HC standards might still be threatened, and in assessing the need for transportation control programs.

No models which attempt to simulate photochemical reactions or the complex distributions of CO in an urban area are included on the list. It has not yet been possible to apply the models developed to simulate these problems in a sufficiently expeditious manner to meet the time demands that are usually expressed. Current models for these problems require such a great deal of computer time or manual manipulation of the input data that it is difficult to consider them as "operational."

It is emphasized that in all cases that are cited, the models were applied to help devise or evaluate an explicit control program. Often, categorical answers were neither needed nor expected. However, a need for a trend, a change in distribution or a range of anticipated air quality levels had been expressed. For these purposes, models, though not perfect, are extremely useful tools in devising programs to enhance the quality of the air environment.

Models are most successfully applied by persons who thoroughly appreciate the model's limitations and who are an integral part of the group which is charged with developing a control tactic. By such means some assurance exists that the most appropriate model for the problem is selected and that the results are used in a manner consistent with capabilities of the model and the quality of the input data.

REFERENCE

1. de Nevers, Noel, "Let's Clear the Air," 36th Annual Reynolds Lecture, Frederick William Reynolds Association, University of Utah, Salt Lake City, February 1973.

Chapter 9

APPLICATION OF IMPLEMENTATION PLANNING PROGRAM (IPP) MODELING ANALYSIS TO THE NEW JERSEY, NEW YORK, CONNECTICUT INTERSTATE AQCR

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FOREWORD

This report presents results of the Implementation Planning Program (IPP) modeling analysis for the New Jersey - New York - Connecticut Interstate AQCR. Results of this study were used in the development and evaluation of the control strategy for this AQCR. The report was originally prepared in draft form in February 1972.

The Monitoring and Data Analysis Division, Office of Air Quality Planning and Standards of the Environmental Protection Agency wishes to thank Messrs. William M. Cox, Russell Lee, Gerald L. Gipson, and Jerome B. Mersch for their efforts in conducting this study.

ABSTRACT

A computer-oriented system has been employed by the Office of Air Programs, EPA, to evaluate the kind and degree of emission control required to achieve the National Primary Air Quality Standards for particulate matter and SO_2 in the New Jersey-New York-Connecticut Air Quality Control Region. The system utilizes an atmospheric diffusion model which simulates the effect of emissions on ground-level pollutant concentrations.

Two control strategies were tested for adequacy in achieving the ambient air quality standards. The first simulated the impact of enforcing proposed regulations, and the results indicated a need for additional control. A second strategy was tested in which natural gas was substituted for residual oil in a zone of high area source emission density.

The major finding of this analysis indicates that the National Primary Air Quality Standards are achievable for both SO_2 and particulate matter, but that moderate increases or redistribution of the usage of natural gas in New York City will be required. The quantity of additional gas required is approximately 90 billion cubic feet per year and represents 20 percent of the gas currently used by the region.

INTRODUCTION

The Clean Air Acts of both 1967 and 1970 require the states to submit an implementation plan which outlines the process by which they will pursue and achieve the goal of clean air. These plans must contain a description of the existing air quality and demonstrate the degree of emission source control that must be obtained to achieve the air quality standards.

To assist the states in developing these control measures, EPA developed, by contract to TRW, a computer-oriented system called the Implementation Planning Program (IPP) which is capable of relating emission rates to air quality, and enables the user to test the impact of various control strategies on pollution levels and on the corresponding regional cost.

As is generally the case with large data systems such as IPP, much time and effort is required to collect and formulate a valid data base. Consequently, many of the states have chosen to use less sophisticated techniques for analyzing the degree of control which they must implement. "Rollback" is the most popular of these techniques and is based on the assumption that an average regional emission reduction will be accompanied by the same percent reduction in pollutant concentrations. Unfortunately, rollback does not allow a detailed consideration of the spatial distribution and height of release of emissions, and is therefore less reliable than the more complex techniques which do consider these factors.

Based on the application of rollback, some rather extraordinary estimates have been made concerning the degree of control which will be required in many of the large complex Air Quality Control Regions. For example, in one application of this technique, it was found that the New York Region would require at least a 200 percent increase in the use of natural gas to meet the National Ambient Air Quality Standards, even though the proposed emission standards are quite stringent for this region.

In view of the rather extreme control measures that the use of rollback indicated would be required in New York as well as in a number of other states, the Office of Air Programs, EPA, began a detailed analysis of the nature and extent of the problem of determining necessary control measures, using the more reliable IPP system. The purpose of this report is to outline the procedures and results of applying the IPP system to data collected for the New Jersey-New York-Connecticut Air Quality Control Region.

II THE SIMULATION MODEL

The following discussion is intended to give a brief summary of IPP. A complete description of IPP can be found in Volume I of the "Air Quality Implementation Planning Program" manual. Several significant changes have been made to this system; these are described in more detail in Appendix A.

The system is composed of a series of interrelated segments that enables the user to proceed through the logical order of (1) relating emission strengths and source locations to ground-level SO_2 and particulate concentrations, (2) testing the overall impact of selected emission reduction schemes (control strategies) on ground-level concentrations, and (3) providing the user with the ability to choose the strategy which assures the attainment of the air quality standards at the least possible cost.

Figure 1 is a schematic representation of the various segments which make this process possible. The source file drives the system; each component of IPP relies on the information that it contains. Emission rates and necessary stack information are input to the air pollutant concentration segment which contains a diffusion model. The diffusion model utilizes this source data along with meteorological data to predict theoretical ground-level concentrations as a function of any set of emission rates. The important output of the air pollutant concentration segment is the source contribution file, which gives the contribution of every emission source to every ground-level receptor.

The source file also serves as an information source for the control strategies segment which is designed to allow the user to impose selected emission standards on various source categories. The effects of these emission control strategies are displayed as expected ground-level concentrations and as emission reductions.

The control strategies segment also makes use of a control cost segment which utilizes the source file in a computation and tabulation of the cost and efficiency of a series of control devices applicable to every source. The control strategies segment uses this information to select the least costly control device that will enable the input emission standard to be met.

The final step in this process is the manual selection of the set of emission limitations which (1) achieves the air quality standards, and (2) does so at the minimum of total regional cost.

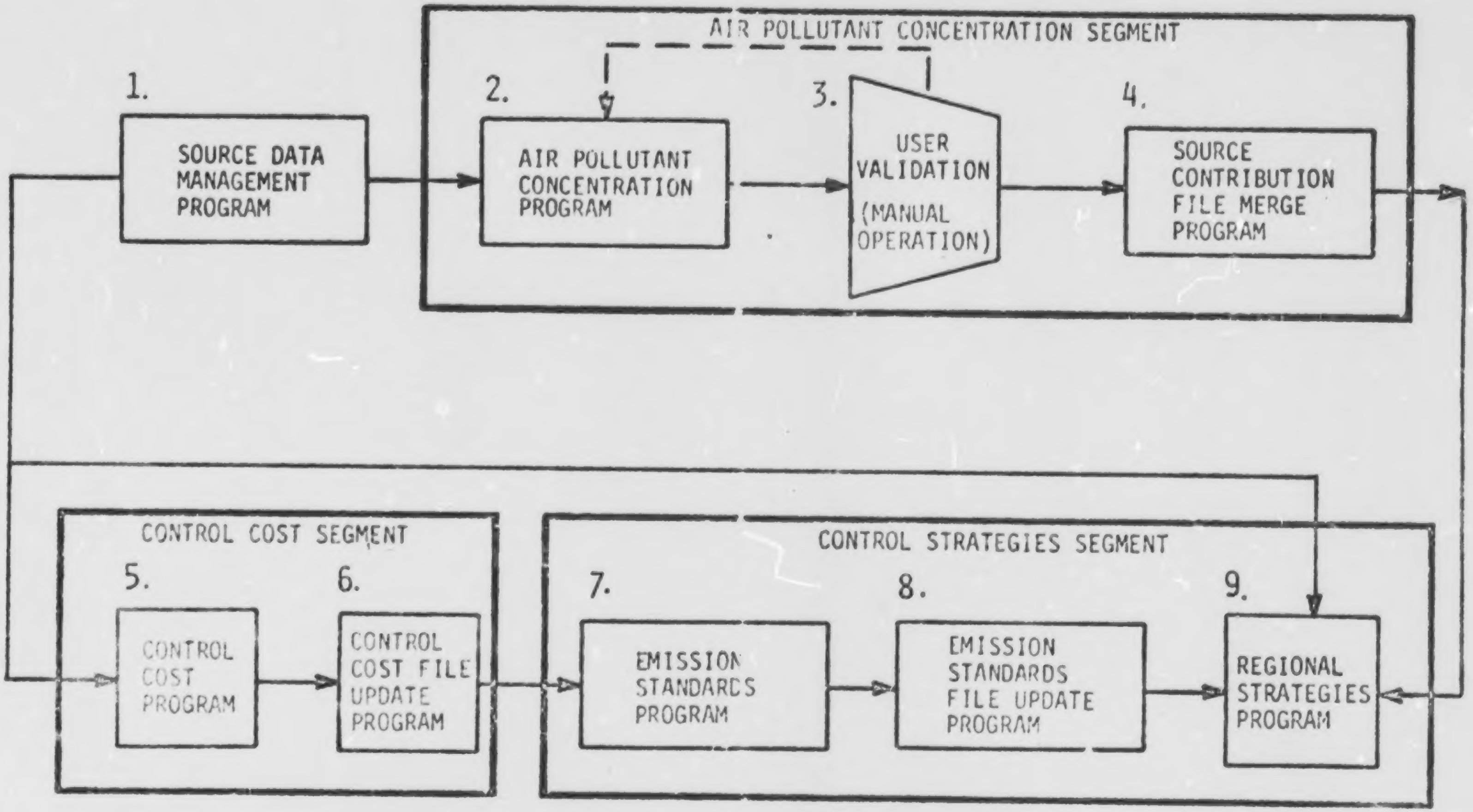
AIR POLLUTANT CONCENTRATION SEGMENT
1.
SOURCE DATA MANAGEMENT PROGRAM
2.
AIR POLLUTANT CONCENTRATION PROGRAM
3.
USER VALIDATION (MANUAL OPERATION)
4.
SOURCE CONTRIBUTION FILE MERGE PROGRAM
CONTROL COST SEGMENT
5.
CONTROL COST PROGRAM
6.
CONTROL COST FILE UPDATE PROGRAM
CONTROL STRATEGIES SEGMENT
7.
EMISSION STANDARDS PROGRAM
8.
EMISSION STANDARDS FILE UPDATE PROGRAM
9.
REGIONAL STRATEGIES PROGRAM

Figure 1. Implementation Planning Program Structure.

III DATA INPUT AND MODEL VALIDATION

Each point and area source of pollutants is considered by the IPP system in its derivation of the theoretical air quality, and its simulation of the effect of emission control strategies. In addition to emission source data, meteorological information must be input in the form of a frequency distribution of selected atmospheric conditions. Another critical input to the system is measured air pollutant concentrations in the form of seasonal or annual averages. These data are used to generate expected ground-level concentrations via a calibrated atmospheric diffusion model. The following subsections describe in detail the input data used for the New Jersey-New York-Connecticut AQCR.

SOURCE DATA

The emissions/source inventory used in this study represents the 1969 calendar year and is an update of the inventory prepared for the 1966 New York abatement conference. It was compiled by the Federal Government in cooperation with the states; the updating was done principally by the states. Regional sulfur oxide emissions decreased by 15 percent from 1966 through 1969 primarily because of restrictions on the sulfur content in fuels that became effective in 1968 in New Jersey and in 1969 in New York. Particulate matter emissions increased by 15 percent during the same period, apparently due to the increase of sources whose total emissions were larger than reductions gained through control measures.

Several significant parameters were collected for each of more than 600 point sources. Some of the more important classes of parameters are listed below.

Source Identification Parameters

- Standard Industrial Classification Code
- Source and Process Type
- (X,Y) Coordinates of Plant or Stack
- Political Jurisdiction

Parameters Affecting Model Estimates of Pollutant Concentrations

- Emission Rates (SO_2 and Particulates)
- Stack Height
- Stack Diameter
- Exit Gas Velocity

Existing Control Equipment Parameters

- Type of Equipment
- Removal Efficiency

Combustion Parameters

- Quantities of Coal, Oil, and Gas
- Sulfur and Ash Contents
- Heating Values

Control Regulation Parameters

- Operating Schedules
- Maximum Boiler Capacity
- Maximum Process Rate
- Maximum Exit Gas Volume
- Maximum Incineration Charge Rate

Considerably less information is required for area sources: an identification number, the size and UTM coordinates, and the average annual emission rate.

METEOROLOGY

The meteorological input to IPP consists of a stability wind rose, the mean afternoon mixing height and the average temperature and pressure for the calendar year 1969.

The stability wind rose used is a joint frequency distribution of 16 wind direction sectors, six wind speed categories, and five Pasquill stability classes. It was derived from measurements collected once every 3 hours at LaGuardia Airport. Although no one set of meteorological data is truly representative of the entire region, LaGuardia data are considered more representative than Newark or Kennedy data for the area of greatest concern, namely Manhattan.

The LaGuardia data, and therefore the model itself, are most accurate for Manhattan, Bronx, northern Queens, northern Brooklyn and the eastern portion of Hudson County. This portion of the region suffers most from the effects of high pollutant concentrations, and hence is of most interest. Nevertheless, the model is considered valid, if somewhat less precise, for the remainder of the region.

Average temperature and station pressure were determined from LaGuardia data. The mean afternoon mixing depth was computed from Kennedy airport upper air data. These three parameters are valid for the entire region.

EXISTING AIR QUALITY AND MODEL CALIBRATION

The final test of any air quality predictive model is a comparison between model estimates and actual monitored pollutant concentrations. This test is accomplished in IPP by a correlative procedure in which observed concentrations are related to computed concentrations by a least squares fit. The sample correlation coefficient between the observed and predicted air quality is computed and compared to a theoretically significant correlation. If the sample correlation is found to be "significant," the least squares procedure is considered statistically valid and all model predictions are adjusted according to the linear regression equation. The model is then said to be "calibrated."

Air quality data representing the 1969 calendar year were obtained from the EPA Regional Office in New York. Particulate matter was monitored by a network of high-volume samplers and results were reported as geometric annual averages. Several analytical techniques were used to monitor for sulfur oxides; each technique was analyzed to determine compatibility with the West-Gaeke (Federal reference) method. Based on data obtained in New York City, an equation was developed to adjust all non-West-Gaeke monitored values to equivalent West-Gaeke results.

Table 1 is a listing of (a) the UTM grid coordinates for each sampling station; (b) the annual averages observed at each monitoring station; and (c) the least squares adjusted values of SO_2. At the bottom of this table are the adjustment equations.

The theoretical ground-level concentrations are determined by employing the diffusion model program portion of the IPP system. A concentration value for both SO_2 and particulate matter is computed for each site at which a monitoring station is located. In addition, concentrations are calculated for a number of arbitrary locations to provide for a more complete regional concentration pattern. The spatial density of these arbitrary sites is increased in areas of highest concentration to assure the inclusion of localized concentration maxima.

Table 1. Air Quality Data Used in the New Jersey-New York-Connecticut Interstate AQCR Study

Annual Averages in μg/m^3

UTM Coord. X	UTM Coord. Y	SO$_2$ Observed	**SO$_2$ Adjusted	Part.	Sampled By	*Method
593.4	4525.5	194	177	92	N.Y. City	(1)
589.5	4517.0	293	267		N.Y. City	(1)
588.7	4519.3	254	231	169	N.Y. City	(1)
592.4	4520.4	280	255	115	N.Y. City	(1)
597.6	4526.6	157	143	95	N.Y. City	(1)
586.8	4513.3	233	212	104	N.Y. City	(1)
592.1	4518.1	207	188	123	N.Y. City	(1)
593.3	4514.6	204	186	117	N.Y. City	(1)
597.9	4516.3	207	188	77	N.Y. City	(1)
601.5	4517.8	154	140	77	N.Y. City	(1)
585.6	4510.1	385	350	112	N.Y. City	(1)
588.9	4509.4	272	248	105	N.Y. City	(1)
592.1	4510.9	178	162	108	N.Y. City	(1)
595.2	4511.9	236	215	94	N.Y. City	(1)
599.7	4510.0	217	198	75	N.Y. City	(1)
602.9	4513.9	162	148	69	N.Y. City	(1)
606.4	4509.8	118	107	71	N.Y. City	(1)
584.1	4500.6	189	172	108	N.Y. City	(1)
585.9	4502.2	283	258	87	N.Y. City	(1)
591.1	4503.6	202	184	84	N.Y. City	(1)
592.1	4507.2	178	162	94	N.Y. City	(1)
595.0	4503.5	165	150	82	N.Y. City	(1)
605.9	4505.8	147	134	67	N.Y. City	(1)
582.1	4496.6	191	174	79	N.Y. City	(1)
588.7	4498.2	210	191	102	N.Y. City	(1)
589.9	4493.9	223	203	77	N.Y. City	(1)
591.1	4500.0	173	158	83	N.Y. City	(1)
599.0	4493.0	118	107	75	N.Y. City	(1)
597.7	4501.3	123	112	75	N.Y. City	(1)
605.0	4502.4	162	148	77	N.Y. City	(1)
569.2	4497.6	178	162	104	N.Y. City	(1)
578.1	4499.3	217	198	95	N.Y. City	(1)
568.0	4491.9	173	158	113	N.Y. City	(1)
573.4	4493.6	181	165		N.Y. City	(1)
576.2	4492.0	162	148	85	N.Y. City	(1)
564.1	4484.2	136	124	80	N.Y. City	(1)
583.3	4509.2	181	165		N.Y. City	(1)
597.4	4521.7	228	208	97	N.Y. City	(1)
615.4	4524.3		45	121	N.Y.State	(2)
615.2	4510.3		82	63	N.Y.State	(2)
613.7	4501.3		47	120	N.Y.State	(2)
604.3	4518.5		77	87	N.Y.State	(2)
608.6	4505.6		77	92	N.Y.State	(2)
614.8	4497.0		53	119	N.Y.State	(2)
606.7	4498.1		84	116	N.Y.State	(2)
609.0	4498.7		65	92	N.Y.State	(2)
620.6	4513.0		63	83	N.Y.State	(2)
630.3	4502.9		47	83	N.Y.State	(2)
620.7	4502.3			88	N.Y.State	
630.5	4495.8		39		N.Y.State	(2)
630.7	4514.8		41	79	N.Y.State	(2)
61[illegible].6	4517.5		37		N.Y.State	(2)

Table 1. (continued)

UTM Coord.		SO_2 Observed	**SO_2 Adjusted	Part.	Sampled By	*Method
X	Y					
590.8	4549.5		43		N.Y.State	(2)
584.7	4555.4		26	55	N.Y.State	(2)
585.3	4567.7		18		N.Y.State	(2)
590.2	4571.4		37	77	N.Y.State	(2)
603.6	4542.7		63	83	N.Y.State	(2)
597.8	4529.5		110	76	N.Y.State	(2)
602.6	4529.0		71	90	N.Y.State	(2)
595.6	4557.0		41	64	N.Y.State	(2)
592.8	4531.6		100	123	N.Y.State	(2)
610.8	4537.7		45	71	N.Y.State	(2)
647.2	4522.7		40		N.Y.State	(2)
660.0	4517.0		36		N.Y.State	(2)
668.7	4516.9		29	100	N.Y.State	(2)
657.9	4531.1		65	57	N.Y.State	(2)
696.7	4531.6		32	42	N.Y.State	(2)
623.0	4525.8			72	N.Y.State	
570.6	4551.7			56	N.Y.State	
612.0	4539.8			70	N.Y.State	
606.8	4532.7			75	N.Y.State	
596.1	4548.5			62	N.Y.State	
600.2	4549.0			54	N.Y.State	
607.6	4573.7			62	N.Y.State	
607.6	4574.2			47	N.Y.State	
600.7	4568.8			42	N.Y.State	
633.5	4510.6			67	N.Y.State	
647.2	4514.5			52	N.Y.State	
644.7	4522.7			58	N.Y.State	
555.5	4484.3	101		67	New Jersey	(3)
579.3	4516.4	90			New Jersey	(3)
565.7	4499.6	103			New Jersey	(3)
574.4	4503.5	147		93	New Jersey	(3)
569.5	4509.6	161			New Jersey	(3)
583.8	4452.1			66	New Jersey	
569.0	4520.3			73	New Jersey	
539.8	4490.1			71	New Jersey	
566.7	4492.5			90	New Jersey	
536.9	4526.4			76	New Jersey	
566.7	4512.4			76	New Jersey	
583.9	4518.3			103	New Jersey	
586.5	4522.5			109	New Jersey	
580.8	4526.1			90	New Jersey	
581.8	4509.9			128	New Jersey	
564.5	4508.6			72	New Jersey	
579.9	4508.7			117	New Jersey	
577.4	4508.8			119	New Jersey	
566.0	4495.4			84	New Jersey	
558.8	4512.6			55	New Jersey	
545.0	4514.5			52	New Jersey	
569.7	4508.9			140	New Jersey	
564.2	4513.0			79	New Jersey	
572.2	4521.2			60	New Jersey	
569.2	4529.5			67	New Jersey	

Table 1. (continued)

UTM Coord.		SO_2	$**SO_2$			
X	Y	Observed	Adjusted	Part.	Sampled By	*Method
560.9	4485.4			78	New Jersey	
579.0	4466.6			61	New Jersey	
543.4	4451.7			51	New Jersey	
562.2	4501.2			84	New Jersey	
547.2	4483.3			62	New Jersey	
554.1	4478.4			90	New Jersey	
532.7	4489.8			68	New Jersey	
580.5	4511.7			95	New Jersey	
582.5	4537.9			63	New Jersey	
651.5	4560.2	173	154	75	Connecticut	(4)
620.9	4545.1	52	46		Connecticut	(4)
622.9	4546.1	115	102	76	Connecticut	(4)
615.7	4542.2	73	65	61	Connecticut	(4)
655.9	4565.2			52	Connecticut	
656.5	4562.1			69	Connecticut	
623.2	4545.5			73	Connecticut	
623.9	4548.3			41	Connecticut	
633.0	4553.3			58	Connecticut	
617.7	4543.7			55	Connecticut	
613.0	4539.7			51	Connecticut	
615.5	4546.0			44	Connecticut	
648.0	4560.7			36	Connecticut	
630.1	4584.1			80	Connecticut	

* 1. H_2O_2
2. Sulfation Plate
3. West Gaeke
4. Conductometric

**H_2O_2 adjusted using Y = .92X
Sulfation Plate adjusted using $((mgSO_4)cm^2 / 30\ day) \times 2.78 \times 0.28 \times 2620 = \mu g/m^3$ of SO
Conductometric adjusted using Y = .89X

The results of calibration are presented in Figures 2 and 3. Both the particulate calibration and SO_2 calibration lines were force-fit by a least squares procedure to a predetermined background value. Based on air quality data obtained from monitoring stations remote from the urban complex, a background value of 35 $\mu g/m^3$ (arithmetic average) was employed for particulate matter. A background of 0.0 $\mu g/m^3$ was assumed for SO_2.

Isopleth maps were prepared using the calibration equations and the theoretical concentrations generated by the diffusion model. The maps which represent annual concentrations for particulate matter and SO_2 in 1969 are presented in Figures 4 and 5, respectively. The patterns are somewhat similar; the maximum concentration for each pollutant appears over Manhattan. Secondary maxima occur in a highly industrialized portion of New Jersey west of Staten Island. Both New York and New Jersey contain significant areas where the primary standard (80 $\mu g/m^3$) is exceeded for both pollutants.

FUEL AND COST INFORMATION

The data used for input to the cost segments of IPP were obtained from two sources: from a private contractor and from the EPA Regional Office in New York. The major aspect of this information is the cost of fuel, not only existing fuel costs by quality, but projected costs as a function of time. Foster Associates of Washington, D. C. were contracted to gather and project fuel cost data for the years 1971 through 1977; their study was intended to provide the price of all fuel types (coal, oil, gas) by quality (sulfur and ash content) and by user type (utilities, industrial, and commercial/residential). The data shown in Table 2 include only the existing (1971) prices of fuels. Thus, the strategies tested and herein reported represent incremental costs that may be incurred if the fuel users were to switch grades or types of fuels at today's prices.

However, because it is based on 1971 prices only, this price structure is unrealistic in the sense that the supply/demand impact of various strategies is not assumed to have any effect on cost of fuels; that is, the 1971-based prices do not consider the differential cost per unit of fuel which may result from two distinct air pollution control policies. For example, this price structure makes no allowance for a price difference that probably would occur between a strategy in which every source is required to switch to low sulfur fuel, and one in which large utilities are allowed to burn high sulfur fuel but use a stack gas desulfurization unit to achieve the required emission standard. Surely, the lower regional demand for low sulfur fuel of the second strategy would result in lower per-unit prices than the high demand requirements of the first strategy in which all users would have to use the same fuel. For these reasons, the values presented for cost of control should be interpreted cautiously.

The remaining input data were collected by the EPA Regional Office in New York. These variables (cost of water, electricity, etc.) were found to contribute little to control costs and will not be further discussed.

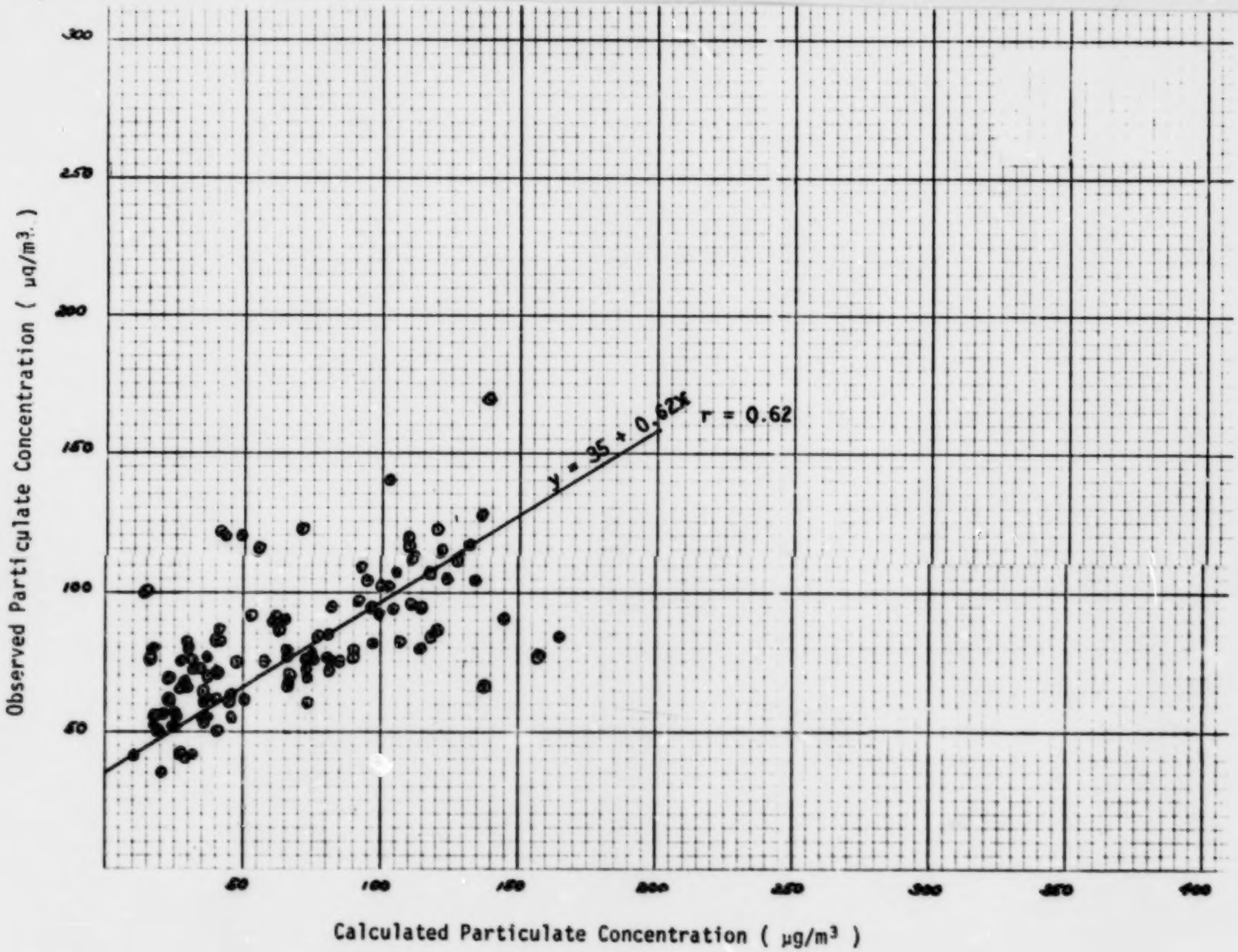

Figure 2. New Jersey-New York- Connecticut Region Particulate Calibration Line

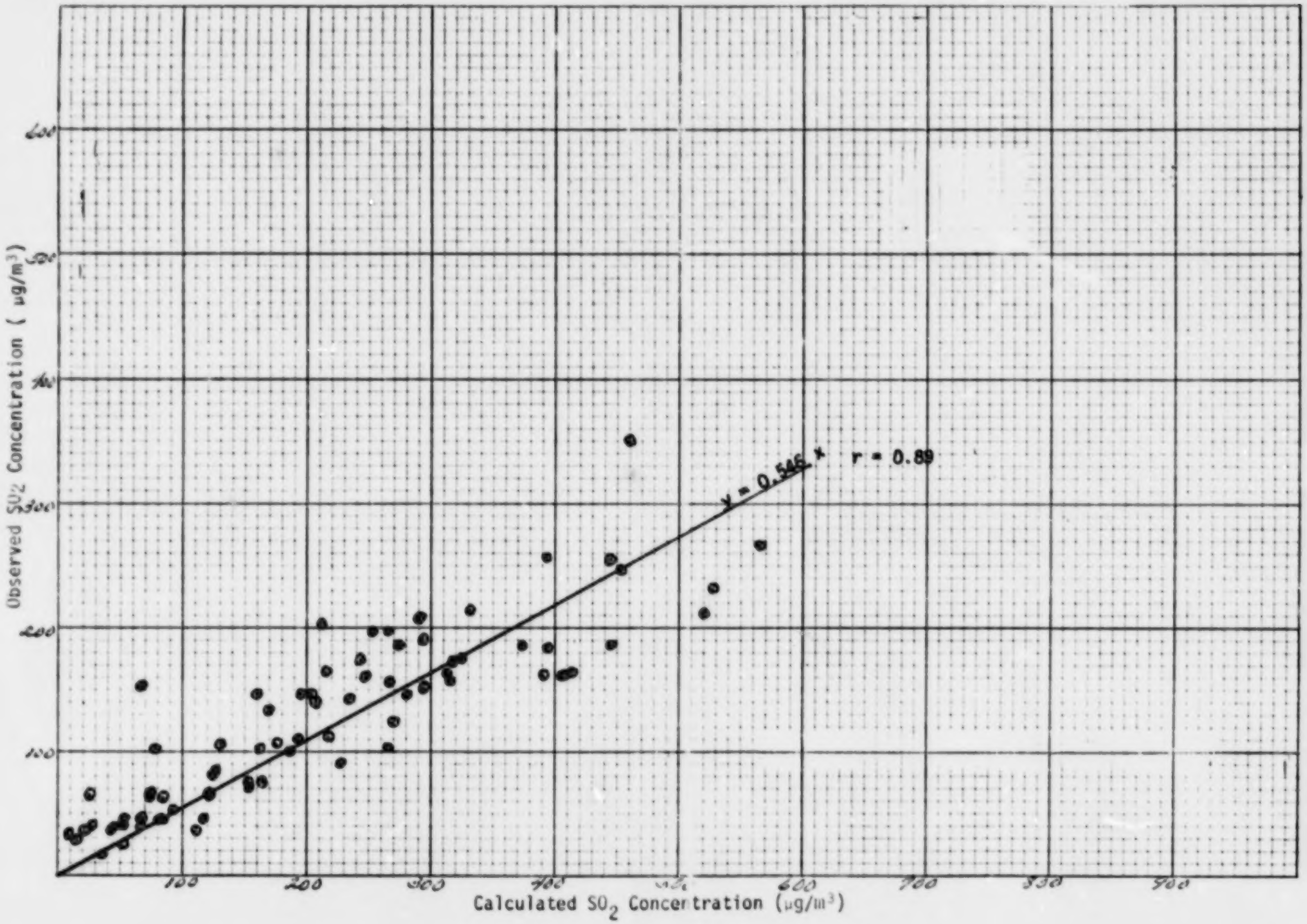

Figure 3. New Jersey-New York-Connecticut Region SO$_2$ Calibration Line

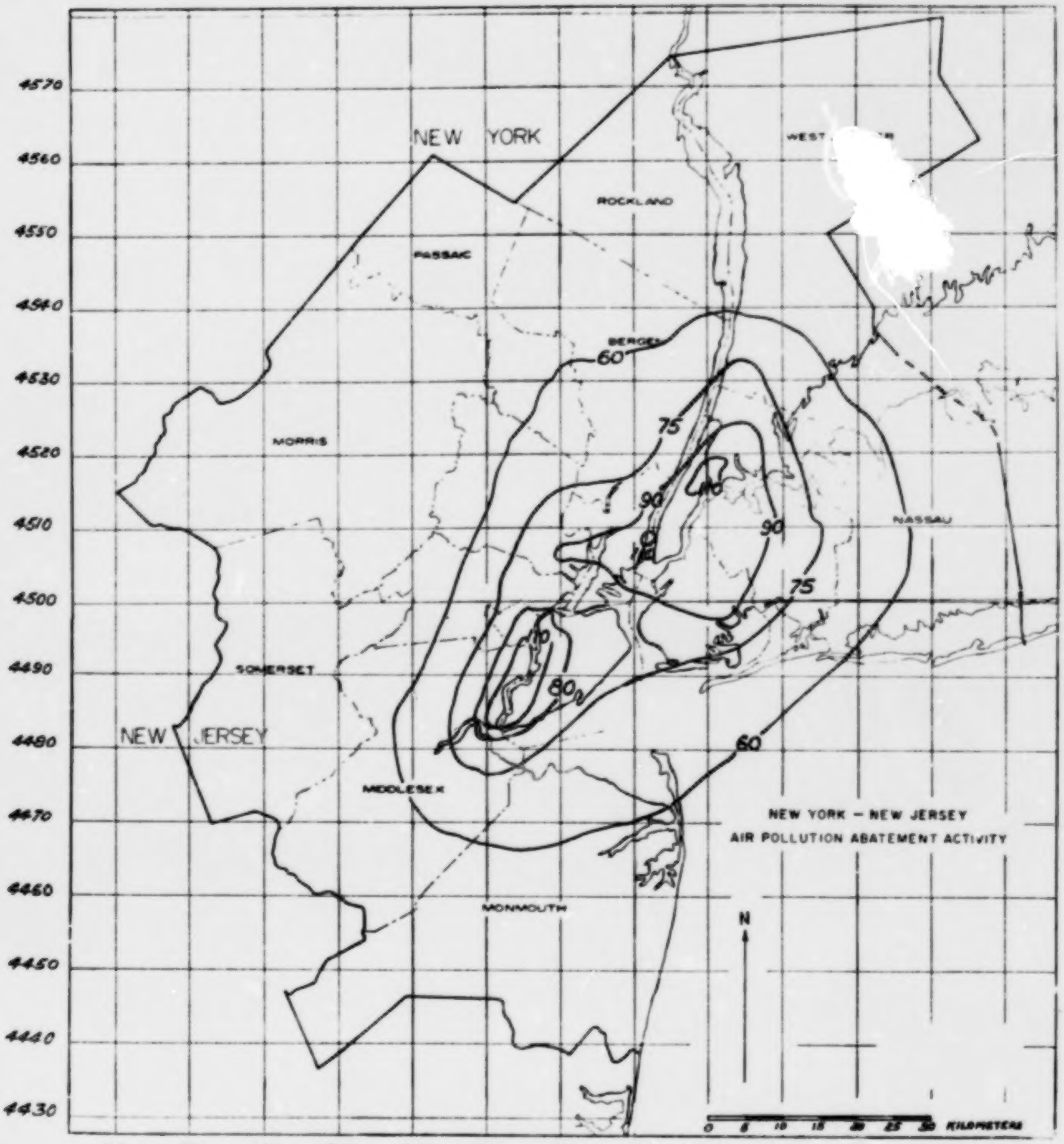
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Figure 4. Current (1969) Model Calibrated Annual Average Particulate Concentration μg/m³

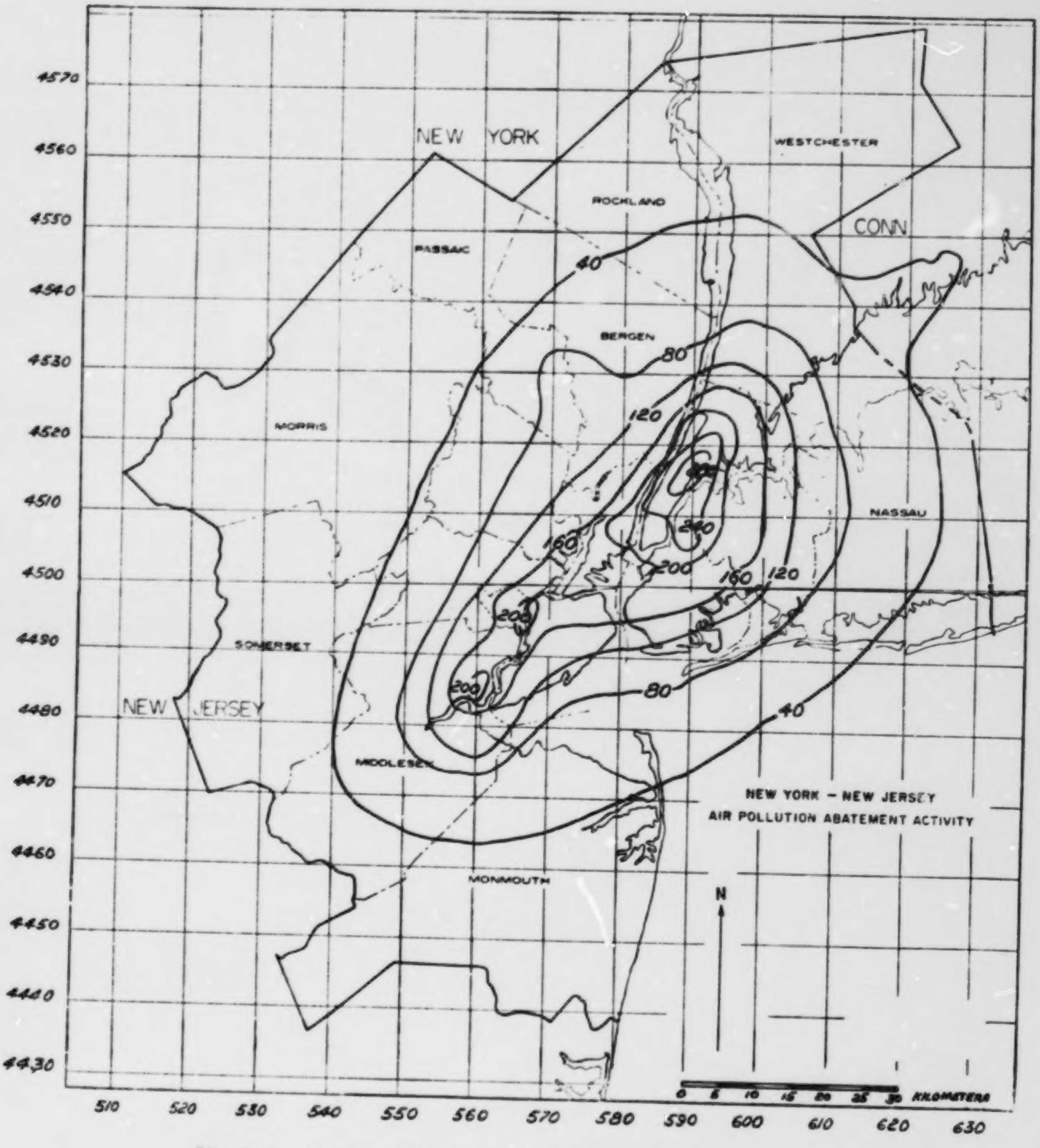
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Figure 5. Current (1969) Model Calibrated Annual Average Sulfur Oxide Concentration $\mu g/m^3$

Table 2. New Jersey-New York-Connecticut Interstate AQCR Regional Cost and Fuel Data

Fuel	Grade	% S Content Max.	% S Content Min.	Heat Content	% Ash Content	Fuel Costs Power Plants	Fuel Costs Industry	Fuel Costs Commercial
Coal	1	1.0	.4	25.5×10^6 BTU/Ton	11.1	$15.32/Ton	$20.16/Ton	$25.01/Ton
	2	1.5	1.0	26.1×10^6 BTU/Ton	9.3	12.25/Ton	17.20/Ton	22.15/Ton
	3	3.0	1.5	24.7×10^6 BTU/Ton	12.7	11.37/Ton	16/06/Ton	21.00/Ton
Residual Oil	1	.5	0	$.148 \times 10^6$ BTU/Gal.		$.105/Gal.	$.130/Gal.	$.176/Gal.
	2	1.01	.5	$.148 \times 10^6$ BTU/Gal.		.083/Gal.	.124/Gal.	.154/Gal.
	3	1.5	1.0	$.148 \times 10^6$ BTU/Gal.		.058/Gal.	.112/Gal.	.129/Gal.
	4	2.6	1.5	$.148 \times 10^6$ BTU/Gal.		.041/Gal.	.071/Gal.	.112/Gal.
Distillate Oil	1	.1	0	$.148 \times 10^6$ BTU/Gal.		$.139/Gal.	$.148/Gal.	$.226/Gal.
	2	.2	.1	$.148 \times 10^6$ BTU/Gal.		.129/Gal.	.138/Gal.	.216/Gal.
	3	.3	.2	$.148 \times 10^6$ BTU/Gal.		.129/Gal.	.138/Gal.	.216/Gal.
Gas	1	0.0		1000 BTU/CU.FT.		$.00115/CU.FT.	$.00119/CU.FT.	$.00158/CU.FT.
Electric Rates						$.0115/KWH	$.0235/KWH	$.034/KWH

Labor Cost - $3.60/Hr.
Water Cost - $.00007/Gal.
Interest Rate - 7.0%

IV CONTROL STRATEGIES

Two control strategies were devised and tested to determine achievability of the National Annual Air Quality Standards for SO_2 and particulate matter. The first of these strategies (Strategy I) simulated the effects of implementing the existing and proposed regulations for the New Jersey-New York-Connecticut AQCR. (These regulations are summarized in Appendixes B and C.) The second control strategy (Strategy II) assessed the additional impact of requiring a portion of area sources in zones of high emission density to switch from the use of residual oil to the consumption of natural gas.

Strategy II was tested because it was found that implementation of the proposed regulations would not be sufficient to achieve the particulate matter standards in Manhattan, and because testing this strategy would illustrate the significant additional improvement that would be achieved in SO_2 air quality.

Before the discussion is continued a few comments should be made concerning the interpretation of these results. The procedure of relating emission rates to ground-level pollution concentration was complex and to a degree uncertain, but was nevertheless considered valid. There were obviously a great number of assumptions which affected this relationship. Throughout the course of the investigation, every attempt was made to ensure a precise and complete emission inventory, but discrepancies and inconsistencies remained. A major assumption was that emissions were uniform throughout the year and that each meteorological condition (wind speed and direction, and atmospheric stability) was representative of the entire region. These assumptions were admittedly tenuous; however, the 1969 relationship between observed and predicted air quality was reasonably good.

Nevertheless, the resulting isopleths of ground-level concentrations must be interpreted with care. Assuming that the estimated concentrations are unbiased, it is possible to make a probabilistic interpretation of estimated concentrations. No specific analysis of errors has been attempted, but it is felt that estimated concentrations should lie within ± 15 to 20 percent of the monitored values.

STRATEGY I

Source Impact - The decrease which would occur in emissions as a result of imposing the existing and proposed regulations on particulates and SO_2 is shown in Tables 3 and 4. Point source reductions were determined by applying the appropriate regulations source by source. All of the controlled emission rates were determined by the IPP system and summed to obtain totals.

The impact of regulations on the reductions in area source emissions was determined externally to IPP and input in the form of scale parameters which were applied to the existing emission rates; for point sources, the impact of regulations was determined directly within the IPP system. An auxiliary computer program was prepared to assist in these calculations. Fuel and emission data supplied by New York were coded according to emission category (Tables 5, 6 and 7). A control matrix corresponding to these emission categories was input to the auxiliary program which estimated the ratio of controlled to existing emissions. These ratios were then processed as input to IPP.

It should be noted that emissions from the "process" and "other" (aircraft, rail, vessels) emission categories have not been listed, primarily because emissions from these categories were relatively small and were not submitted to EPA by New York State. Furthermore, proposed control measures

Table 3. Effects of Current and Proposed Regulations on Particulate Emissions

Source Category	1969 Emissions (tons/day)	Controlled Emissions (tons/day)	% Reductio
New York			
Fuel Combustion	87.64	37.24	58
Industrial Process	0	0	0
Solid Waste	86.72	15.49	82
Area Sources	224.70	170.80[1]	24
State Total	399.06	223.53	44
Connecticut			
Fuel Combustion	12.62	11.72	7
Industrial Process	1.06	0.51	52
Solid Waste	4.02	3.95	2
Area Sources	11.50	11.50	0
State Total	29.20	27.68	5
New Jersey			
Fuel Combustion	88.45	26.99	69
Industrial Process	59.91	5.11	91
Solid Waste	1.38	0.55	60
Area Sources	172.90	110.90	36
State Total	322.64	143.55	44
Regional Summary			
Fuel Combustion	188.71	75.95	60
Industrial Process	60.97	5.62	91
Solid Waste	92.12	19.99	78
Area Sources	409.10	293.20	28
Region Totals	750.90	394.76	47

[1] Controlled emissions were further reduced to 150.1 tons/day by Strategy II.

Table 4. Effects of Current and Proposed Regulations on SO_2 Emissions

Source Category	1969 Emissions (tons/day)	Controlled Emissions (tons/day)	% Reduction
New York			
Fuel Combustion	654.06	138.65	79
Industrial Process	0	0	0
Solid Waste	11.61	11.61	0
Area Sources	1019.60	209.00[1]	80
State Total	1685.27	359.26	79
Connecticut			
Fuel Combustion	393.77	181.27	54
Industrial Process	0	0	0
Solid Waste	.33	.33	0
Area Sources	26.10	26.10	0
State Total	420.20	207.70	51
New Jersey			
Fuel Combustion	659.68	140.87	79
Industrial Process	85.73	48.76	43
Solid Waste	.32	.32	0
Area Sources	887.60	460.70	48
State Total	1633.33	650.65	60
Regional Summary			
Fuel Combustion	1707.51	460.79	73
Industrial Process	85.73	48.76	43
Solid Waste	12.26	12.26	0
Area Sources	1933.30	695.80	64
Region Totals	3738.80	1217.61	67

[1] Controlled emissions were further reduced to 166.0 tons/day by Strategy II.

Table 5. Area Source Emission Summary for Manhattan

	Particulate Emissions		SO$_2$ Emissions	
	Tons/Year	Percent	Tons/Year	Percent
ANTHRACITE COAL				
Industrial	15	0.1	10	Neg.
Residential	874	5.5	3763	3.3
Commercial	834	5.3	539	0.5
BITUMINOUS COAL				
Industrial	0	0	0	0
Residential	17	0.1	55	0.1
Commercial	453	2.9	292	0.2
DISTILLATE OIL				
Industrial	362	2.3	1704	< 1.5
Residential	462	2.9	3262	2.9
Commercial	540	3.4	2543	2.3
RESIDUAL OIL				
Industrial	1866	11.8	22926	20.3
Residential	3315	21.0	40732	36.1
Commercial	2878	18.2	35365	31.3
NATURAL GAS				
Industrial	41	0.3	1	Neg.
Residential	69	0.5	1	Neg.
Commercial	82	0.5	2	Neg.
TRANSPORTATION				
Gasoline	1849	11.7	1387	1.2
Diesel	920	5.8	335	0.3
ON-SITE INCINERATION	1218	7.7		0
PROCESS	Not Reported	-	Not Reported	-
OTHER (Aircraft, Rail, Vessels)	Not Reported	-	Not Reported	-
Total	15,795	100.0	112,917	100.0

Table 6. Area Source Emission Summary for Bronx

	Particulate Emissions		SO_2 Emissions	
	Tons/Year	Percent	Tons/Year	Percent
ANTHRACITE COAL				
Industrial	11	0.2	7	Neg.
Residential	354	5.9	1523	4.4
Commercial	359	6.0	231	0.7
BITUMINOUS COAL				
Industrial	0	0	0	0
Residential	10	0.2	32	0.1
Commercial	239	4.0	154	0.4
DISTILLATE OIL				
Industrial	56	0.9	263	0.8
Residential	602	10.1	4247	12.2
Commercial	207	3.5	971	2.8
RESIDUAL OIL				
Industrial	165	2.8	2030	5.8
Residential	1294	21.6	15896	45.6
Commercial	712	11.9	8745	25.1
NATURAL GAS				
Industrial	8	0.1	0	0
Residential	71	1.2	1	Neg.
Commercial	24	0.4	0	0
TRANSPORTATION				
Gasoline	800	13.4	600	1.7
Diesel	407	6.8	148	0.4
ON-SITE INCINERATION	660	11.0	0	0
PROCESS	Not Reported	-	Not Reported	-
OTHER (Aircraft, Rail, Vessels)	Not Reported	-	Not Reported	-
Total	5,979	100.0	34,848	100.0

Table 7. Area Source Emission Summary for Brooklyn

	Particulate Emissions		SO_2 Emissions	
	Tons/Year	Percent	Tons/Year	Percent
ANTHRACITE COAL				
Industrial	0	0	0	0
Residential	622	5.4	2676	4.2
Commercial	963	8.3	623	1.0
BITUMINOUS COAL				
Industrial	0	0	0	0
Residential	11	0.1	34	0.1
Commercial	353	3.0	228	0.3
DISTILLATE OIL				
Industrial	198	1.7	934	1.5
Residential	1329	11.5	9382	14.7
Commercial	514	4.4	2419	3.8
RESIDUAL OIL				
Industrial	929	8.0	11407	17.9
Residential	1994	17.3	24502	38.4
Commercial	817	7.1	10036	15.7
NATURAL GAS				
Industrial	99	0.9	2	Neg.
Residential	324	2.8	7	Neg.
Commercial	148	1.3	3	Neg.
TRANSPORTATION				
Gasoline	1617	14.0	1213	1.9
Diesel	928	8.0	337	0.5
ON-SITE INCINERATION	711	6.2	0	0
PROCESS	Not Reported	-	Not Reported	-
OTHER (Aircraft, Rail, Vessels)	Not Reported	-	Not Reported	-
Total	11,557	100.0	63,803	100.0

would not significantly affect emissions from these two categories; therefore, such emissions were excluded from area source analysis.

For area source fuel combustion it was assumed that the very stringent coal sulfur regulations that have been proposed for New York and New Jersey would result in the eventual elimination of coal as a fuel. The only exception to this assumption would be in New Jersey, where regulations would allow domestic sources to continue to burn 0.7 percent sulfur coal. However, considering the trend toward the elimination of coal usage, it was assumed that 50 percent of the domestic coal users would switch to oil.

Other reductions in area source emissions would come from the impact of regulations in the categories of on-site incineration and from the indirect effect of regulations intended to eliminate lead in gasoline. On-site incineration particulate emissions would likely decrease by 33 percent; the anti-lead regulations would result in a 50 percent reduction in emissions of particulate matter from gasoline-powered vehicles. A summary of the assumptions concerning area source reductions is given in Table 8.

Comparison of Tables 9 and 10 indicates the impact of Strategy I on fuel consumption by source category.

Air Quality Impact - The expected annual ground-level concentrations resulting from Strategy I are shown in Figures 6 and 6A for particulates and Figures 7 and 7A for SO_2. Most areas in New Jersey would probably achieve the particulate matter National Primary Ambient Air Quality Standard of 75 $\mu g/m^3$ (geometric mean). Most of Manhattan and large portions of the Bronx, Queens, and Brooklyn would likely remain over the standard. Maximum

Table 8. Area Source Strategy Assumptions

STRATEGY I

- No Growth
- Assumes a 50% reduction in particulate emissions from transportation sources to reflect anti-lead regulations.
- Assumes a 33% reduction in particulate emissions from on-site incineration.
- Stringent sulfur regulations will result in coal being replaced by fuel oil with the exception that only 50% of the domestic users in New Jersey will switch because of less stringent sulfur regulations (0.7%) for these users.
- Assumes 1969 Area Source Fuel Sulfur Content as:

	Ant. Coal	Bit. Coal	Residual Oil	Dist. Oil
New York	1.7	1.7	1.8	0.45
New Jersey	0.7	1.0	1.0	0.40

- Assumed Coal Ash Content of 7.5%.

STRATEGY II

- Same as Strategy I except all coal in chosen high emission density grids to gas.
- 50% of residual oil in chosen grids to gas.

Table 9. New Jersey-New York-Connecticut Interstate AQCR
Fuel Summary for the Base Year 1969

Political Jurisdiction	Point Sources	Area Sources	Total
New York			
Coal (Tons/Day)	12,526	1,095	13,621
Residual Oil (1,000 Gal./Day)	1,777	4,603	6,380
Distillate Oil (1,000 Gal./Day)	3,524	4,701	8,225
Gas (10^6 CU.FT./Day)	9	527	536
New Jersey			
Coal (Tons/Day)	8,791	5,001	13,792
Residual Oil (1,000 Gal./Day)	4,398	173	4,571
Distillate Oil (1,000 Gal./Day)	13	4,310	4,323
Gas (10^6 CU.FT./Day)	156	327	483
Connecticut			
Coal (Tons/Day)	4,612	0	4,612
Residual Oil (1,000 Gal./Day)	1,179	61	1,240
Distillate Oil (1,000 Gal./Day)	1	115	116
Gas (10^6 CU.FT./Day)	0	--	0
Regional Summary			
Coal (Tons/Day)	25,929	6,096	32,025
Residual Oil (1,000 Gal./Day)	7,354	4,837	12,191
Distillate Oil (1,000 Gal./Day)	3,538	9,126	12,664
Gas (10^6 CU.FT./Day)	165	854	1,019 1/

1/ Information obtained from the Region II Office indicates that the total regional gas usage is closer to 1400 X 10^6 cubic feet per day. The difference is primarily due to unreported interruptible gas used by many of the utilities listed in the IPP source file.

Table 10. New Jersey-New York-Connecticut Interstate AQCR

Fuel Summary for Control Strategy I and II

Political Jurisdiction	Point Sources	Area Sources	Total
New York			
Coal (Tons/Day)	0	0	0
Residual Oil (1,000 Gal/Day)	4,091	4,701 1/	8,792
Distillate Oil (1,000 Gal/Day)	3,484	4,806 2/	8,290
Gas (10^6 CU.FT./Day)	9	527 3/	536
New Jersey			
Coal (Tons/Day)	0	344	344
Residual Oil (1,000 Gal/Day)	6,098	582	6,680
Distillate Oil (1,000 Gal/Day)	13	4,748	4,761
Gas (10^6 CU.FT./Day)	156	327	483
Connecticut			
Coal (Tons/Day)	4,699	-- 5/	4,699
Residual Oil (1,000 Gal/Day)	1,203	61	1,264
Distillate Oil (1,000 Gal/Day)	1	115	116
Gas (10^6 CU.FT./Day)	0	-- 5/	0
Regional Summary			
Coal (Tons/Day)	4,699	344	5,043
Residual Oil (1,000 Gal/Day)	11,392	5,344	16,736
Distillate Oil (1,000 Gal/Day)	3,498	9,669	13,167
Gas (10^6 CU.FT./Day)	165	854	1,019 4/

1/ For Strategy II, 3,200 10^3 Gal/Day of Residual Oil.

2/ For Strategy II, 4,733 10^3 Gal/Day of Distillate Oil.

3/ For Strategy II, 762 10^3 CU.FT./Day of Natural Gas.

4/ See footnote 1 in Table 9.

5/ Values not reported.

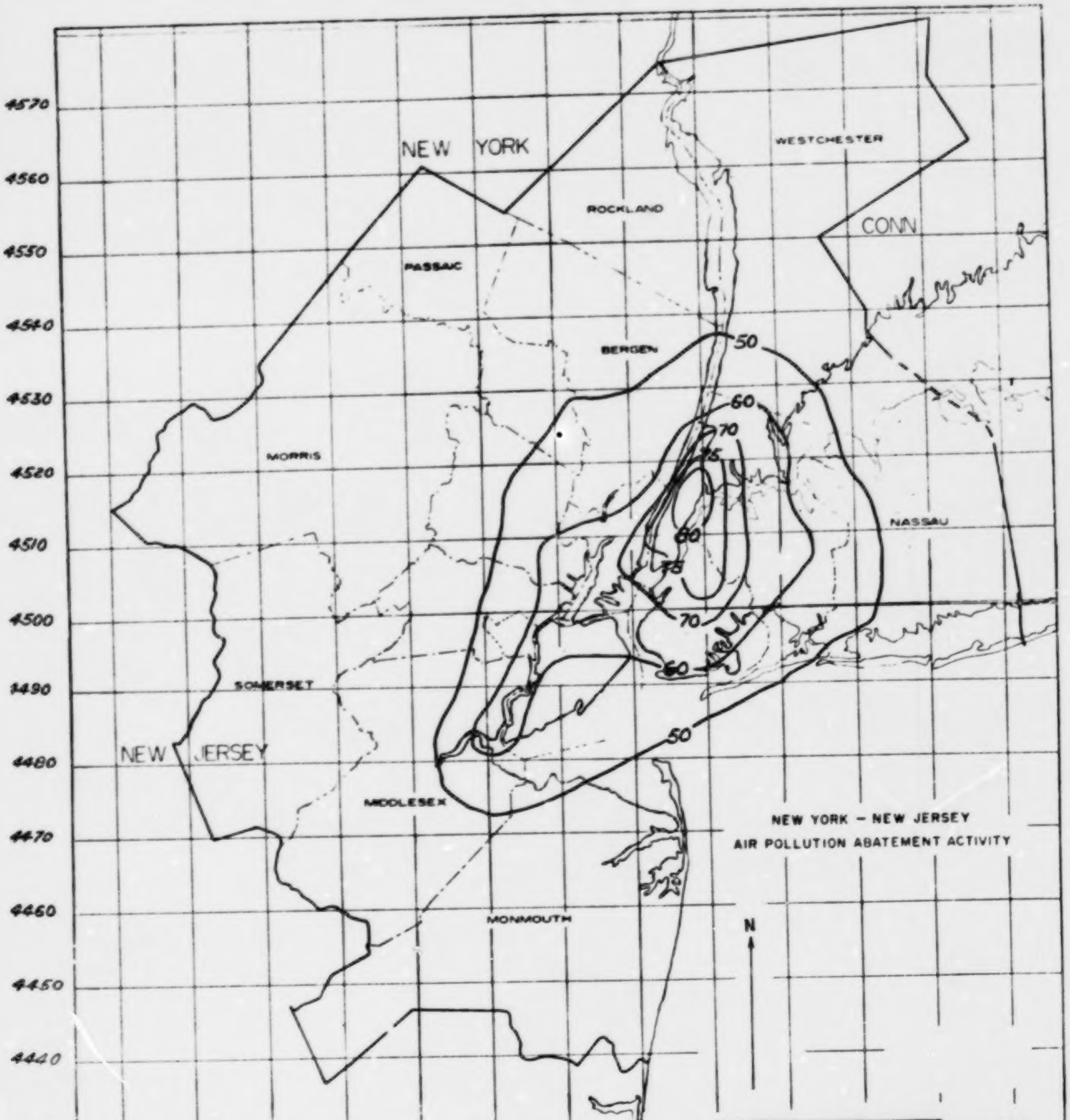
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Figure 6. Strategy I - Particulates, μg/m³

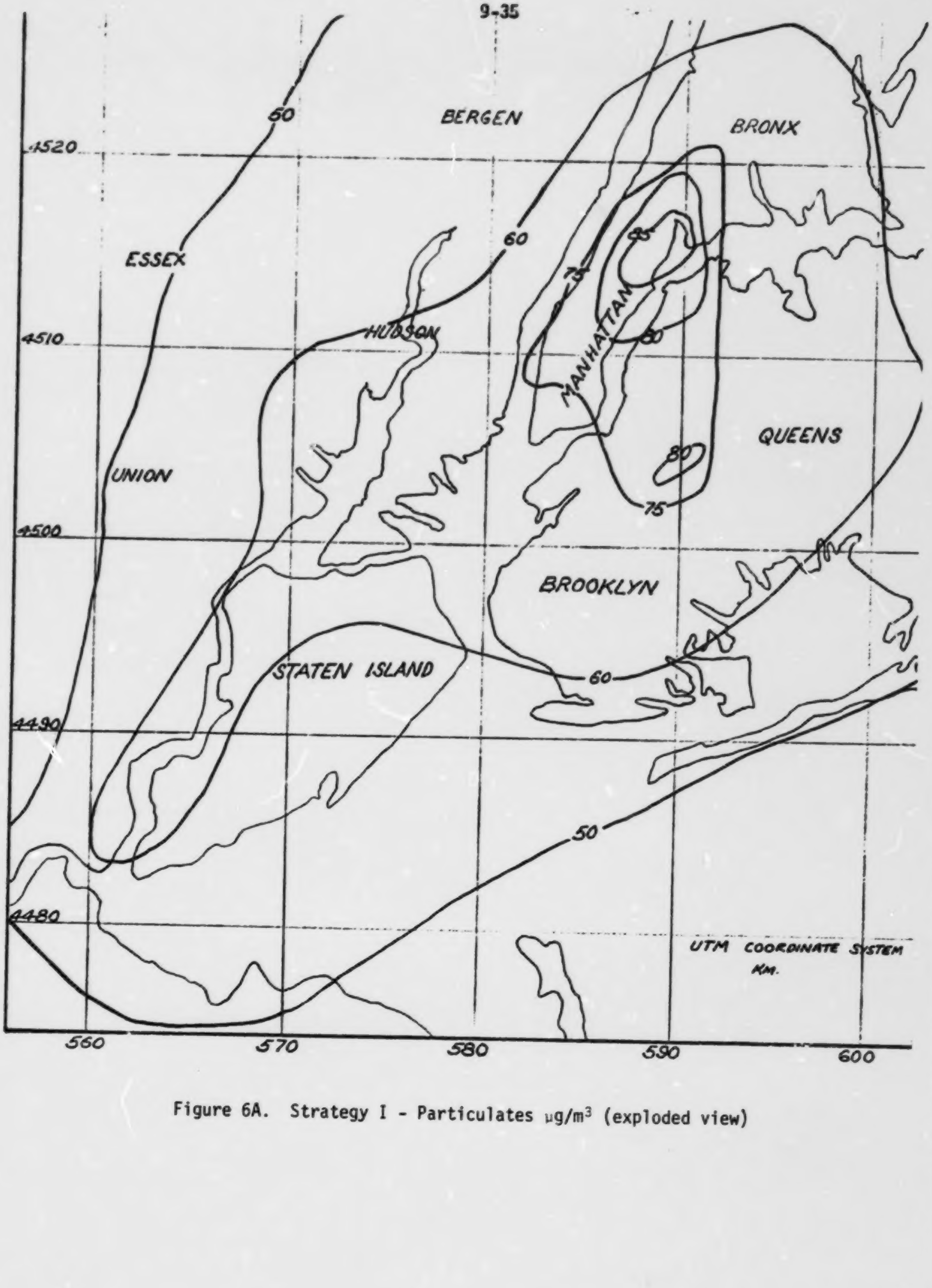
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Figure 6A. Strategy I - Particulates μg/m³ (exploded view)

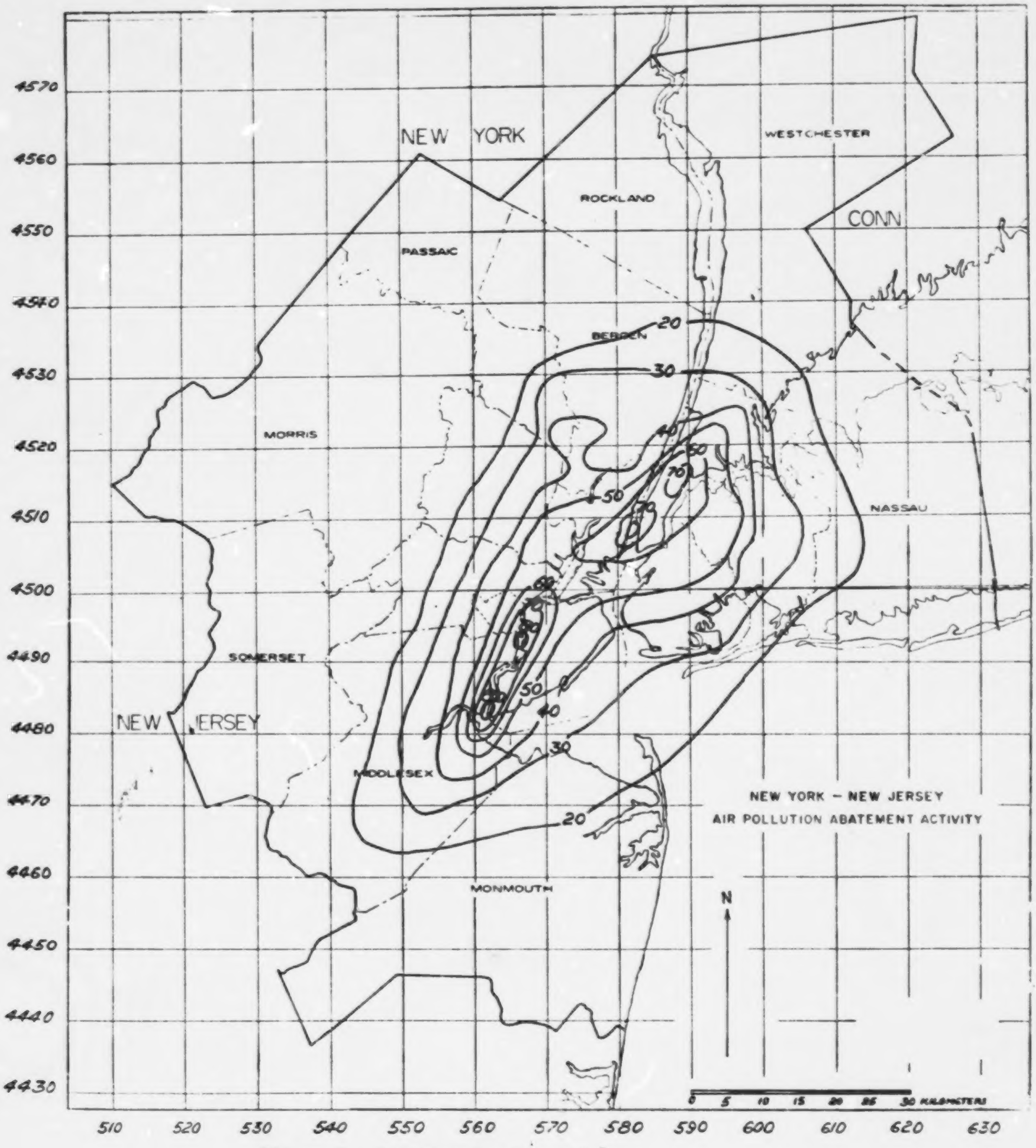
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Figure 7. Strategy I - SO_2 μg/m^3

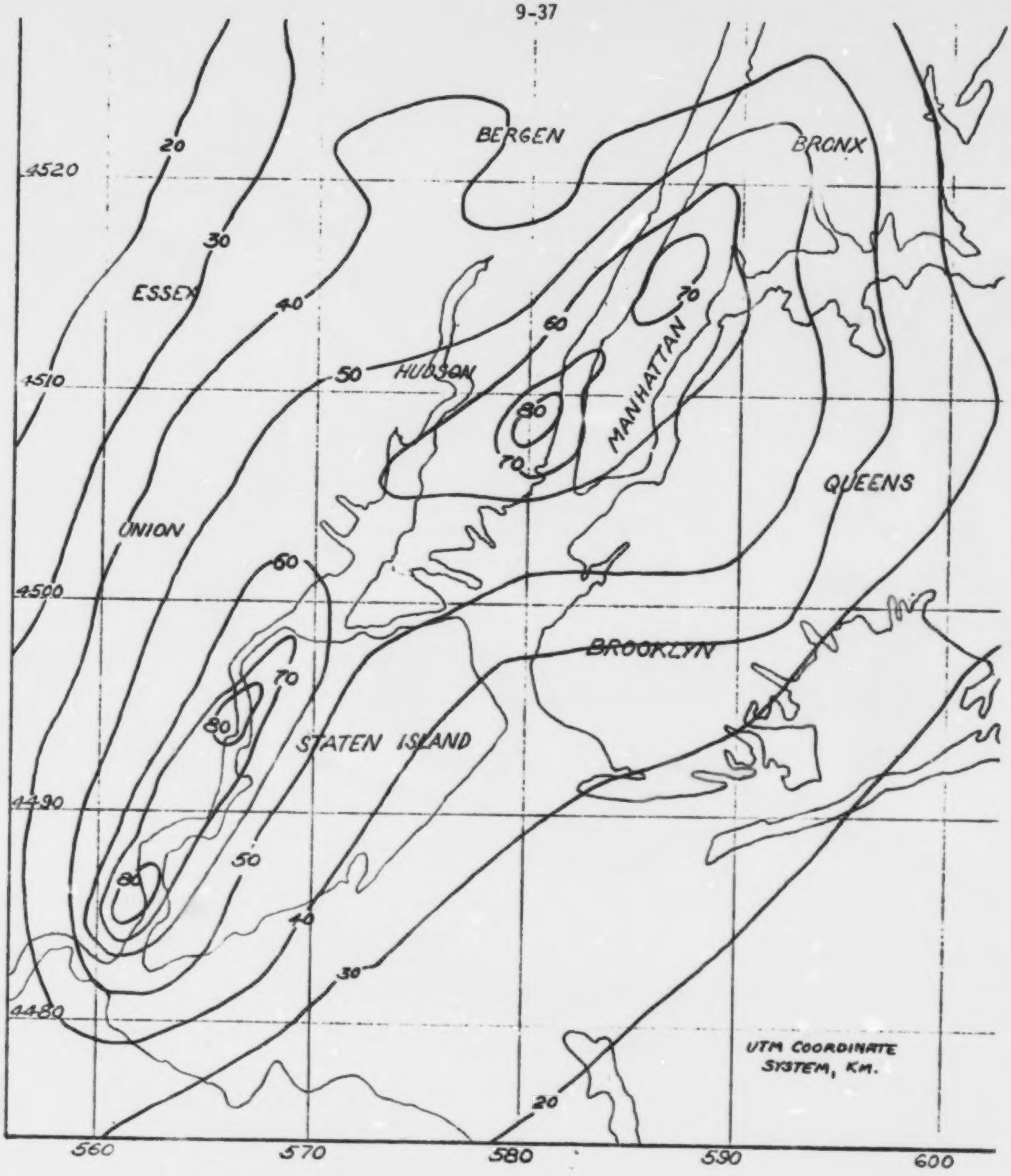

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Figure 7A. Strategy I - SO_2, µg/m³ (exploded view)

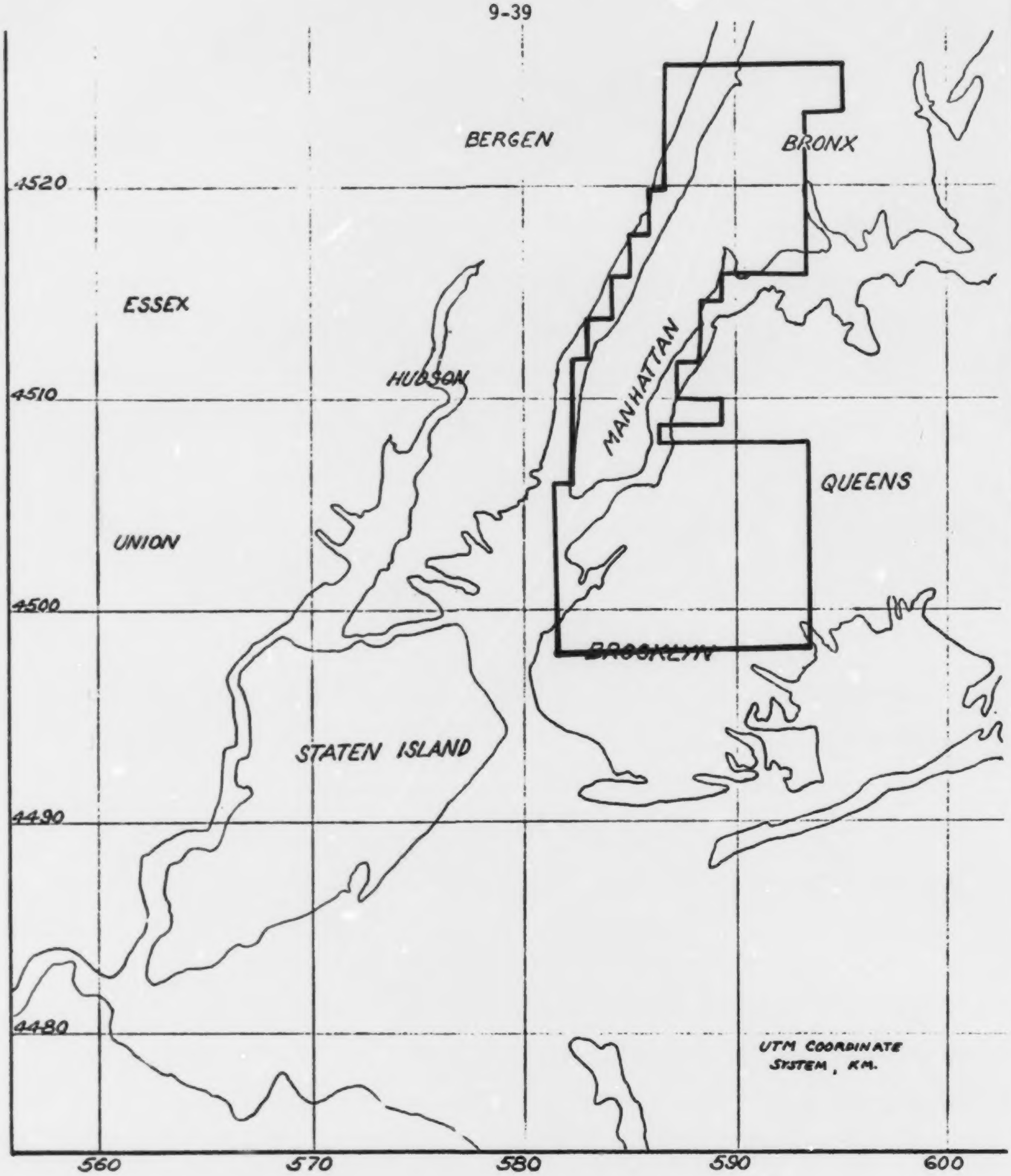
concentrations would probably occur over northern Manhattan and portions of the Bronx, where concentrations would approach 90 $\mu g/m^3$.

The projected SO_2 pattern would be similar to that of particulates. The notable exception is that the primary standard would not be exceeded over New York City, but that local maxima exceeding the primary standard would occur in Jersey City and in parts of Middlesex and Union Counties. All of these maximum concentrations would be near 85 $\mu g/m^3$, which indicates that additional SO_2 control would probably be required in New Jersey. For example, if the New Jersey process code for SO_2 were tightened from 2000 ppm to 500 ppm (and if this tightened 500 ppm code were enforced), the SO_2 primary standard would be achieved throughout the New Jersey portion of the Region.

The impact of existing and proposed regulations would likely result in air quality over Connecticut which would be well within the primary standards for both particulates and SO_2.

STRATEGY II

Source Impact - The only sources affected by Strategy II, as compared to Strategy I, would be those area sources consuming coal and residual oil in certain high emission density grids in Manhattan, the Bronx, and Brooklyn. Figure 8 shows the location of these grids. An examination of the relative contribution to total particulate and SO_2 emissions from the various area source categories led to the choice of Strategy II. The contributions are presented from Manhattan, the Bronx, and Brooklyn in Tables 5, 6 and 7, respectively.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4500
BROOKLYN
STATEN ISLAND
4490
4480
UTM COORDINATE SYSTEM, KM.
560
570
580
590
600

Figure 8. Zone of High Area Source Emission Density

The majority of both the SO_2 and particulate emissions in 1969 resulted from the burning of residual oil in these three boroughs. In Manhattan residual oil accounted for 51 percent of all area source particulate emissions, and for nearly 90 percent of the SO_2 emissions. A first attempt to reduce these emissions might be made by converting the residual oil to a cleaner oil, such as distillate. However, current literature on emission factors shows that switching from residual to distillate oil will result in only a 30 percent reduction in particulate emissions - a reduction insufficient to allow the achievement of the air quality standard.

An alternate strategy was tested in which 50 percent of the residual oil and all coal burning would be replaced by an equivalent consumption of natural gas; this strategy would require a gas increase of 86 billion cubic feet per year. This amount represents an approximate 30 percent regional increase in gas usage. There are unquestionably problems with the implementation of such a fuel conversion, especially in light of the national shortage of gas. But no other alternatives appear more feasible at this time.

It should be noted, however, that an annual conversion from residual oil to gas consumption is not the only method of implementing this strategy. Equivalent results could be obtained if the required quantity of gas could be transferred from warm season users, such as utilities, to selected area source users in the zone of high emission density during the heating season. In either case, pipeline and shortage capacities would probably require expansion to meet the increased load. These problems are currently being investigated.

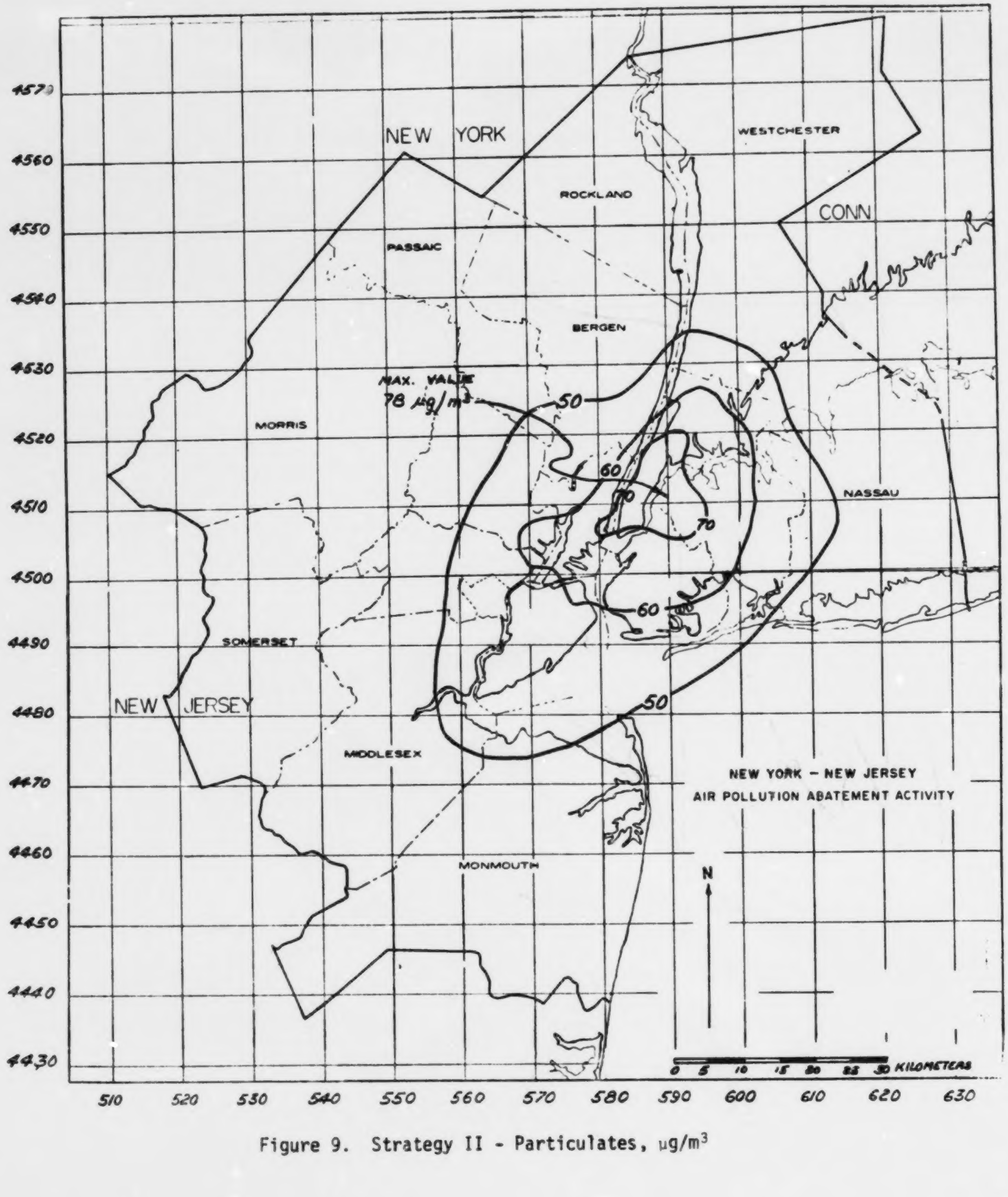
Air Quality Impact - Figures 9, 9A, 10, and 10A show the impact of Strategy II on particulate and SO_2 air quality. The maximum particulate value would still occur at the same location in Manhattan, but would drop to 78 μg/m³ (geometric mean); this drop indicates that the particulate primary standard would quite possibly be achievable. The land area above standard would significantly decrease. Most of the three boroughs would meet the standard; only a localized problem area would remain.

An even greater improvement is noted in the SO_2 air quality. The concentration reduction in New York and particularly in Manhattan would be large enough to meet the secondary standard of 60 μg/m³ throughout the most of the New York portion of the region. Only a small area in central Manhattan would have any problem in achieving this standard.

In New Jersey, the only location where the increased gas usage in New York would significantly reduce SO_2 concentrations is at the site of the maximum in Jersey City, where SO_2 concentrations would be further reduced by approximately 10 percent.

COST OF CONTROL

Annualized control costs may be divided into two parts: (a) those which would occur because of the requirement for cleaner fuels, and (b) those which would occur because of the purchase and operation of mechanical devices. It was found that the former category would dominate the cost of control in the New York Region, based on the fuel cost data obtained from Foster Associates. Table 11 presents a summary of these costs for both point and area sources for each control strategy. The total regional cost of implementing Strategy I would be 282 million dollars; all but 7 million dollars would be attributable to the increase in clean fuels. The cost to area sources of implementing this strategy would be nearly as large as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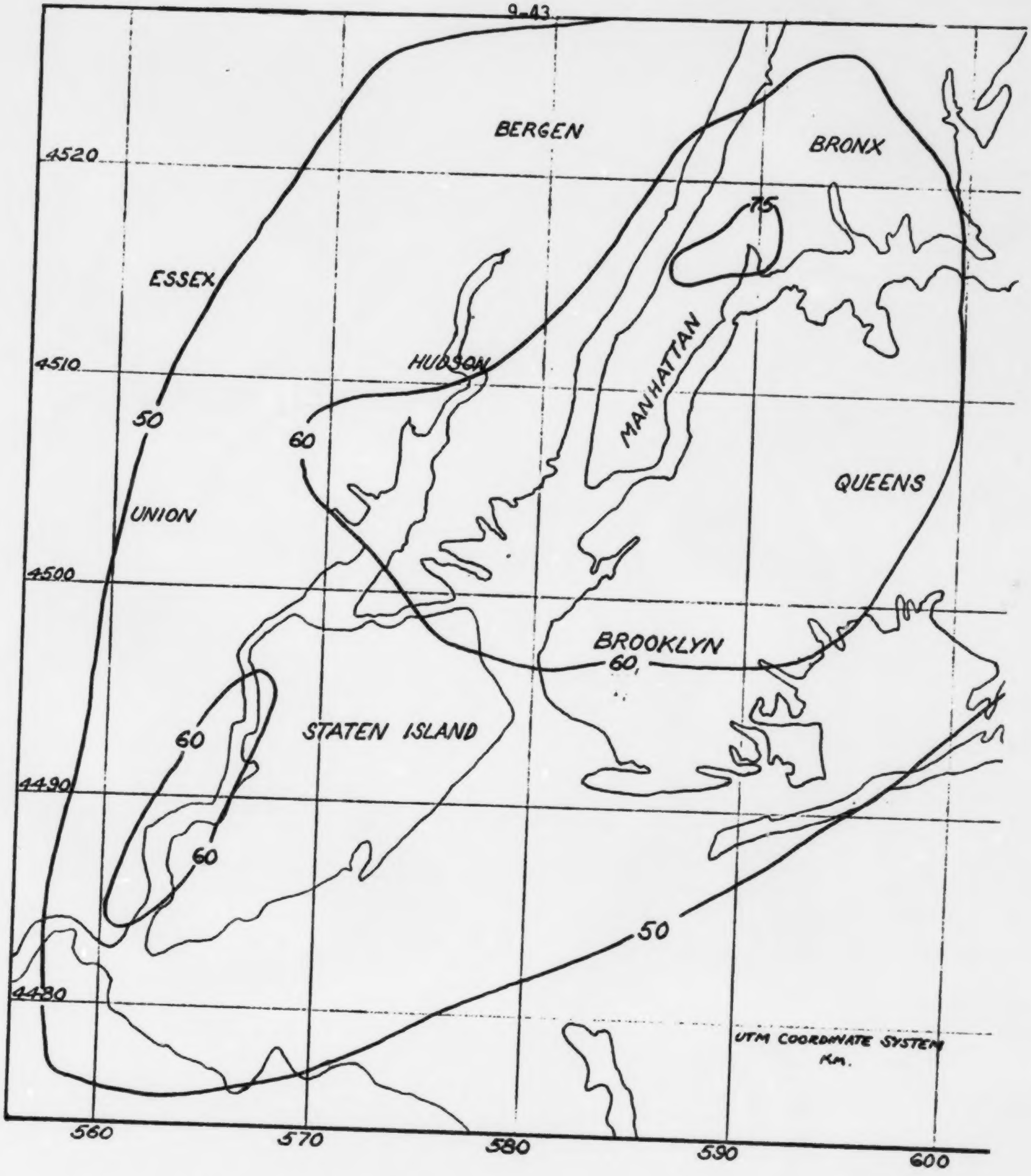
630
NEW YORK
WESTCHESTER
ROCKLAND
CONN
PASSAIC
BERGEN
MAX. VALUE
78 µg/m³
50
60
70
70
60
50
MORRIS
NASSAU
SOMERSET
NEW JERSEY
MIDDLESEX
NEW YORK – NEW JERSEY
AIR POLLUTION ABATEMENT ACTIVITY
MONMOUTH
N
0 5 10 15 20 25 30 KILOMETERS

Figure 9. Strategy II - Particulates, µg/m³


BERGEN
BRONX
ESSEX
HUDSON
MANHATTAN
QUEENS
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BROOKLYN
STATEN ISLAND
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UTM COORDINATE SYSTEM
Km.

Figure 9A. Strategy II - Particulate, μg/m³ (exploded view)

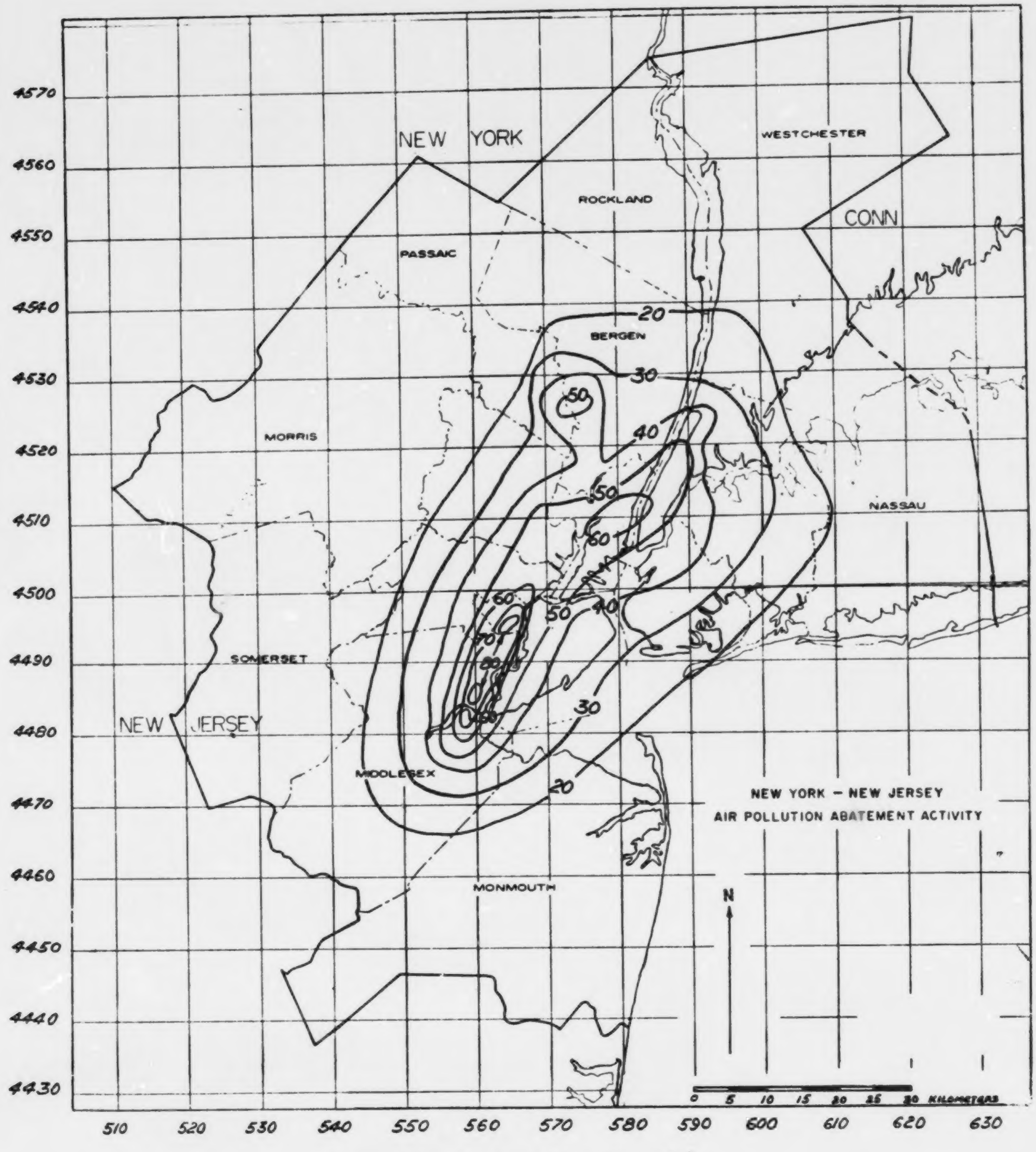
NEW YORK
WESTCHESTER
ROCKLAND
CONN
PASSAIC
BERGEN
MORRIS
NASSAU
SOMERSET
NEW JERSEY
MIDDLESEX
MONMOUTH
NEW YORK – NEW JERSEY
AIR POLLUTION ABATEMENT ACTIVITY
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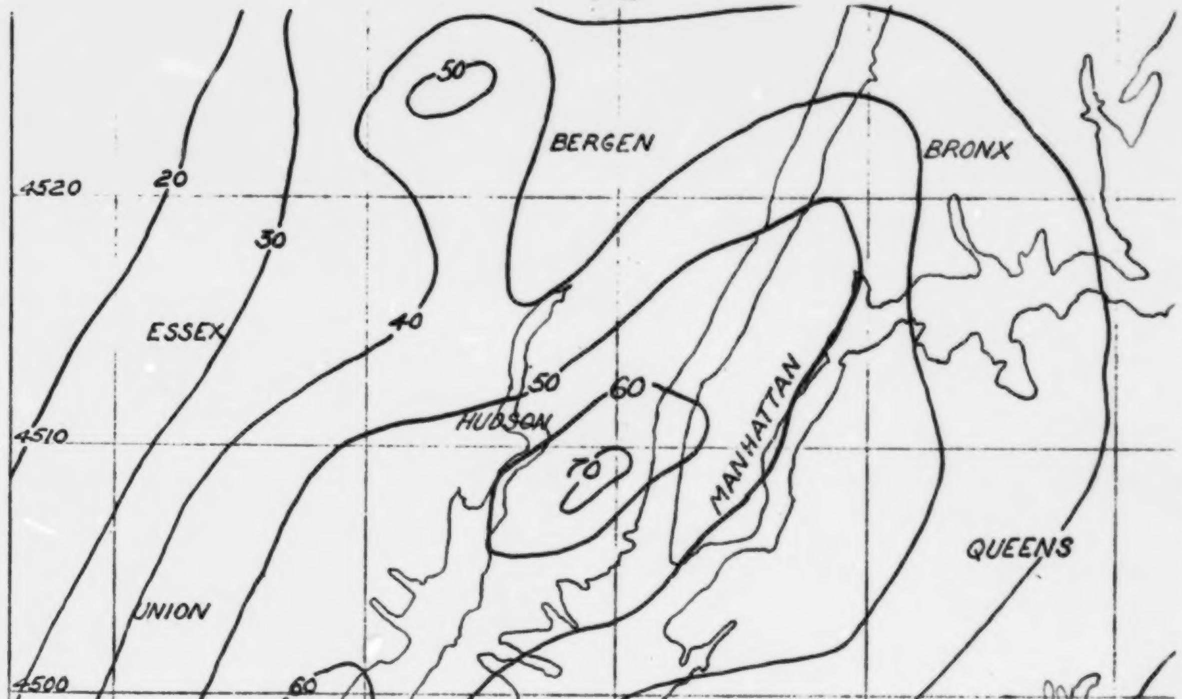
Figure 10. Strategy II - SO_2 μg/m³


BERGEN
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UTM COORDINATE
SYSTEM, KM.

Figure 10A. Strategy II - SO_2, $\mu g/m^3$ (exploded view)

Table 11. New Jersey-New York-Connecticut Interstate AQCR Cost Summary (in millions of dollars)

	Point Sources Annual Cost	Area Source Strategy I Cost	Total Cost (Point & Area)
New York			
Fuel Switching	58.4	129.2[1/]	187.6
SO_2 Mechanical Devices	0	0	0
Particulate Mechanical Devices	2.2	0	2.2
New Jersey			
Fuel Switching	51.0	9.3	60.3
SO_2 Mechanical Devices	0.2	0	0.2
Particulate Mechanical Devices	4.5	0	4.5
Connecticut			
Fuel Switching	26.3	1.2	27.5
SO_2 Mechanical Devices	0	0	0
Particulate Mechanical Devices	0.1	0	0.1
Region			
Fuel Switching	135.7	139.7	275.4
SO_2 Mechanical Devices	0.2	0	0.2
Particulate Mechanical Devices	6.8	0	6.8
Totals	142.7	139.7	282.4

1/ Add 29.5 million dollars for Strategy II to reflect higher cost of natural gas.

that for point sources. This projected cost reflected the large prices of cleaner fuels; no cost of mechanical devices was considered for area sources.

The additional cost of implementing Strategy II would be nearly 30 million dollars and would apply only to area sources in Manhattan and in the previously described grids in the Bronx and Brooklyn. This cost reflected the added expense of converting coal and 50 percent of the residual oil to natural gas at today's fuel prices. Note in Table 11 that no attempt was made to assess the cost of boiler conversion or the cost of increased gas distribution capacity.

Also not shown in Table 11 is the fact that approximately 80 percent of the cost of control would be incurred by power plants which would have to switch from high-sulfur coal and residual oil to low-sulfur fuel oil.

Certainly worthy of future examination is the economic assessment of stack gas desulfurization for power plants versus a clean fuel requirement for all sources; such an examination can be conducted once a realistic fuel supply/demand model has been demonstrated and the cost and efficiency of stack gas desulfurization devices are better established.

V UTILIZATION OF RESULTS

A primary purpose of this effort was to provide information on the nature and severity of control required to achieve the air quality standards in the New Jersey-New York-Connecticut Interstate AQCR. OAP agreed to supply these results to EPA Region II office and to the state air pollution control agencies in order to establish a mutual understanding of the control that may be required. To this end, a series of meetings and presentations was scheduled. The first meeting, held in the New York Regional Office, was to permit OAP to explain to the Regional Office and to the states why OAP was conducting a modeling study of the Region, and to invite participation by the states. OAP agreed to furnish the states copies of the output; of particular interest was the source contribution file. The state representatives felt that this information would assist them in the development of their implementation plans for SO_2 and particulate matter. Emission control regulatins were discussed and it was decided that the existing and proposed regulations of each state would be tested. If these regulations would not achieve the standards, OAP agreed to test additional emission reduction schemes and forward the results.

During October, the State of New Jersey informed the Regional Office that New Jersey could not achieve the primary standard for particulate matter. The Regional Office suggested to the state that the results of the New York modeling study be used in New Jersey's implementation plan in lieu of the state's calculations, which were based on rollback. New Jersey agreed to use the IPP results which indicated that the primary standards for particulates were achievable.

Several presentations were made to staff personnel of OAP in Durham to highlight the analytical capabilities of IPP and to demonstrate the necessity for limited increases in natural gas usage in New York City. A significant fact which emerged from these presentations was that area sources represent an extremely large contribution to ground-level receptors; this fact served to illustrate the need for EPA consideration of a "clean fuel" policy.

In December, the Regional Office again requested the assistance of the Source Receptor Analysis Branch (SRAB) in the preparation given to a selected group of New York legislators who were concerned with progress being made in the control of air pollution. Based on results of IPP, charts were prepared and displayed which demonstrated the pollutant concentrations which could be achieved by implementing the proposed emission regulations. It was also pointed out that natural gas may have to replace some of the fuels currently used in central portions of New York City. An additional purpose of this meeting was to demonstrate the degree of cooperation being exercised among the Federal and State Governments and to illustrate the resulting progress in developing satisfactory state implementation plans for the achievement of the National Ambient Air Quality Standards.

Based on the generally favorable response to the capabilities of IPP, it is recommended that the system be used to assist the states in determining the degree of control that will be required to achieve the National Secondary Air Quality Standards. The greatest benefit would accrue to those states which have asked for the 18-month extension for submission of the implementation plan to achieve these standards. Ample time would be available for close regional/state cooperation with the Office of Air Programs and would allow a closer examination and upgrading of input data.

APPENDIX A

Utilization of the IPP system by OAP had lead to several improvements in its adequacy and flexibility. A number of errors have been detected and corrected; these corrections required considerable manpower. Several of the programs concerned with the application of emission limitations were partially recoded to enable them to perform as the IPP manual describes. These programs included: (1) a standard which would allow a least cost selection between a fuel switch alternative or flue gas desulfurization, (2) an emission standard which would limit stack gas concentration on a volumetric basis, (3) an emission standard which would limit mass emission rate per unit volume of gas flow, and (4) a similar standard limiting the mass emissions per mass of exhaust gas. In addition, several changes were made to portions of the IPP system which deal with SO_2 emissions from sulfur-bearing fuels. IPP was incorrectly assigning the sulfur content limitation.

Several auxiliary programs were written which enhanced the usefulness of the source contribution file. A series of programs was prepared which allowed the user to modify this file by source or receptor. These modifications made possible the correction of source impact on ground-level concentrations without rerunning the entire diffusion model, and resulted in a savings of nearly 50 hours of computation. Additional programs centered around the source contribution file were prepared and included (1) a program which listed the concentration contributions of the three highest contributors for each receptor, (2) a program which summarized the contribution of area and point sources at each receptor, (3) a program which accumulated contributions within preselected Standard Industrial Classification Codes, and (4) a program which printed the source contribution file for selected receptor sites.

APPENDIX B

Proposed and Existing Particulate Control Regulations in the New Jersey-New York-Connecticut AQCR

A. New York

1. Fuel Combustion. The following table applies to the control of particulate matter from the combustion of solid fuel:

Total Heat Input, 10^6 BTU/hr.	Max. Wt. Discharge, lb./hr.
1	.6
10	6
100	37
1,000	225
10,000	1,360

For heat inputs not listed above, use log-log interpolation. Because of the severe sulfur limitation of 0.3 percent placed upon coal, it was assumed that all coal burners will switch to fuel oil.

2. Industrial Process. There are no point sources in New York City affected by the state emission standard.

3. Solid Waste. The following standard applies to the control of particulate matter from incinerators:

Process Weight, lb/hr.	Max. Wt. Discharge, lb/hr.
1	.002
1,000	2.00
20,000	26.7
100,000	82.2

For process weights not listed above, use log-log interpolation. For Westchester and Rockland Counties, the maximum weight discharge is equal to 0.5 percent of the process weight.

B. Connecticut

1. Fuel Combustion. The following table applies to the control of particulate matter from the combustion of fossil fuels:

Total Heat Input, 10^6 BTU/hr.	Max. Wt. Discharge, lb/hr.
1	.6
10	6
10,000	1,200
100,000	12,000

For heat inputs not listed above, use log-log interpolation.

2. Industrial Process. The following table applies to the control of particulate matter from industrial process sources:

Process Wt. Rate, lb./hr.	Max. Wt. Discharge, lb./hr.
100	.55
1,000	2.58
10,000	12.00
100,000	44.60
1,000,000	69.00
6,000,000	92.7

For process weight rates not listed above, use log-log interpolation.

3. Solid Waste. A particulate emission standard of .4 lb. of particulates per 1,000 lb. of exhaust gas is applied to incinerators.

C. New Jersey

1. Fuel Combustion. The following table applies to the control of particulate matter from the combustion of solid fuel:

Total Heat Input, 10^6 BTU/hr.	Max. Wt. Discharge, lb./hr.
1	0.6
10	6.0
200	20.0
1,000	100.0
10,000	1,000.0

For heat inputs not listed above, use log-log interpolation. Because of the severe sulfur limitation of 0.2 percent placed upon coal, it was assumed that all coal burners will switch to fuel oil.

2. Industrial Process. The following table applies to the control of particulate matter from industrial process sources:

Potential Emissions, lb./hr.	Max. Wt. Discharge, lb./hr.
50 or less	.5
100	1.0
1,000	10.0
2,000	20.0
3,000 or greater	30.0

For potential emissions not listed above, use log-log interpolation.

3. Solid Waste. The following table applies to the control of particulate matter from incinerators:

Process Weight	Max. Grain loading value
Less than 2,000 lb./hr.	0.2 grains/SCF
2,000 lb./hr.	0.2 grains/SCF
Greater than 2,000 lb./hr	0.1 grains SCF

APPENDIX C

Proposed and Existing SO_2 Control Regulations in the New Jersey-New York-Connecticut AQCR

A. New York

1. Fuel Combustion. The following table applies to the sulfur content of fuel burned in New York:

Fuel	Max. Sulfur Content, % S by weight
Coal	0.3%
Residual Oil	0.3%
Distillate Oil	0.1%

Because of the severe sulfur limitation of 0.3 percent placed upon coal, it was assumed that all coal burners will switch to fuel oil.

2. Industrial Process. There are no point sources in New York City affected by the state emission standard.

3. Solid Waste. No standard.

B. Connecticut

1. Fuel Combustion. The following table applies to the sulfur content of fuel burned in Connecticut:

Fuel	Max. Sulfur Content, % S by weight
Coal	1.0%
Residual Oil	1.0%
Distillate Oil	1.0%

2. Industrial Process. No standard.

3. Solid Waste. No standard.

C. New Jersey

1. Fuel Combustion. The following table applies to the sulfur content of fuel burned in New Jersey:

Fuel	Max. Sulfur Content, % S by weight
Coal	0.2%
Residual Oil	0.3%
Distillate Oil	0.2%

Because of the severe sulfur limitation of 0.2% placed on coal, it was assumed that all coal burners will switch to fuel oil.

2. Industrial Process. An SO_2 emission standard of 2,000 parts per million is applied to industrial process sources.

3. Solid Waste. No standard.

Addendum to Modeling Analysis of the New Jersey-New York-Connecticut AQCR

The natural gas strategy (Strategy II) was tested to determine the impact of a slight modification in natural gas distribution in New York City. This modification reflects no additional gas (above Strategy I requirements) to area sources in Brooklyn, but reflects a 70 percent residual oil gas replacement (instead of 50 percent) to area source users in Manhattan and the Bronx. The total gas usage required by this modification remained about the same as Strategy II and would require an additional 86 billion cubic feet per year over current usage.

The air quality impact is to further reduce the area of particulate concentration maxima located over Manhattan. The station of maximum concentration would drop from 78 $\mu g/m^3$ to 75 $\mu g/m^3$, thus technically allowing the achievement of the national primary standard. Since the background concentration of 35 $\mu g/m^3$ was assumed, this 3 $\mu g/m^3$ decrease in concentration at the maximum site represents about a 7 percent increase in nonbackground air quality.

Particulate matter air quality over Brooklyn would not suffer appreciably as a result of this modification. The maximum site in Brooklyn for Strategy I was 80 $\mu g/m^3$. The concentration at this station would fall to 75 $\mu g/m^3$ for Strategy II compared to 76 $\mu g/m^3$ for the modified Strategy II. Apparently the large increase in gas usage in Manhattan and the Bronx would adequately reduce the concentration at this receptor in Brooklyn.

A similar result is found for SO_2. Since it appears that the secondary standard will be met throughout New York City, the results will not be discussed.

Because this modified gas strategy allows the primary standard to be achieved over Manhattan and at every other site in New York City (except the indicated site at 76 $\mu g/m^3$), it is recommended as a better alternative to Strategy II. Furthermore, this modification may be easier to implement because fewer boroughs would be involved.

Chapter 10

USE OF DISPERSION MODELS DURING PLANNING PHASES OF INDUSTRIAL AND DOMESTIC REGIONS

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

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Use of Dispersion Models during Planning Phases of Industrial and Domestic Regions.

V. Meeting of
NATO/CCMS
June, 4. - 6. 1974
Roskilde, Denmark

Use of Dispersion Models during Planning Phases of Industrial and Domestic Regions

Social and political background

For the decision of land use as defining industrial and residential regions, respectively, and in deciding the expansion or the settlement of industrial plants it is of strong importance that no significant injury or molestation due to industrial air pollution is induced. To check the air quality situation to be expected in the exceptional case, the administration demands for an air quality forecast around the plant. Such a prognosis is, in general, ordered by the administration and carried out by federal institutions as the LIB 1) or by private institutions as for instance the TÜV 2).

These experts firstly need the emissions situation to be expected due to the plant parts to be settled and secondly the real basic pollution load of the region. The emissions situation is described by emissions inventories / 1 /; an emissions inventory is a detailled and complete listing of all sources of air pollution substances, classified according to their geographical source position and the conditions affecting the emissions like source dimensions, quantity of pollutants, frequency and duration of emissions etc.

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1) LIB = Landesanstalt für Immissions- und Bodennutzungsschutz, an institution of the country of Northrhine-Westfalia, dealing with problems on air pollution and air quality.

2) TÜV = Technischer Überwachungs-Verein, supervising institutions, being engaged with air pollution problems, too.

Concerning the futurous residential settlement it is of course difficult or even impossible to give a hypothetical emissions inventory of domestic heating emissions because in most cases the detailled use of an area of immission cannot be described previously.

The procedure for industry is more clear because complete detailled data on emissions and emission conditions have to be given by the industry during the licensing procedure. On the basis of such an emissions declaration a hypothetical emissions inventory can be derived.

The new "Bundesimmissionsschutz-Gesetz", a new law in action since April 1st 1974 in the Fed. Rep. of Germany demands for instance

1. for emission inventories in strongly industrialized areas and
2. for emissions declarations in industrialized zones , at least, and
3. for an updating every year.

Due to the directions of this new law it is of great importance, especially, in the case of the licensing procedure to state by an air quality forecast, wether the planned plant will cause toxic or molestic influences to the environment or not. The limits of injurious environmental effects of pollutants are given by air quality standards, i.e. maximum immission concentration values.

The prognosis of air pollution to be expected around the plant due to the plant becomes more and more important because the settlement of the plant cannot be licensed without the proof that it will not effect environmental influences.

The task of the experts now is the calculation of air pollution concentrations. Such calculations are possible on the basis of mathematical - meteorological dispersion models using existing or hypothetical emissions inventories. The prognoses comprise a large varity of substances or groups of components and it has to take into account the already existing basic load.

Experience has shown that the diverse models used for forecasts as well as the numerous dispersion parameters not necessarily yield the same results even using quite equivalent conditions. The state as licensing authority, however, must look upon the unique handling and deciding. It cannot be tolerated that such important decisions as the licensing of industrial plants depend on either the expert or the model used or the parameters selected.
In order to get identical criteria of the prognoses the Minister of Labour, Health and Social Affairs of North-rhine-Westfalia is discussing to proclaim a standardized guideline for the execution of the air quality forecast, that has to be followed by the licensing authority as well as by the experts. By this, similar licensing facts should be handled and decided similarly in our country.

The state authority therefore sees himself as user of the models, although he himself does not executes the calculations.
It is evident that making such a guideline for the forecast both modelers and users have to be involved in the development. By this development dispersion models are passed over from the phase of scientific discussion to the phase of practical use. Its importance cannot be valuated high enough, as often the prognostic calculation is the basis for the license of a project of some millions' or even a billion's value. Deciding for "Yes" or "No" this instrument gains a heavy responsability. The scientific discussion on setting up and developping models as well as parameters, therefore, must take this fact into account.

During this phases of model application in our country we see the difficulties in standardizing the models. The following part of the paper will present some of the difficulties to be solved and the aim and hope is to get some suggestions for the continuation of our work during this meeting.

Dispersion model used

In a few words a brief scope of the model used for the calculations around plants to be expanded or plants to be settled is given; see also / 2, 3 /:

The model uses the well known formula with gaussian distributions horizontally and vertically. The diffusion parameters used should be valid for regions of a certain roughness due to industrial plants, urban areas or else. Calculations are done for gaseous pollutants only and the pollution components do not suffer neither physical or chemical changes in the atmosphere nor an absorption at the ground. Plume rise is calculated using the formula given by Moses and Kraimer / 4 /, it takes into account the dynamic and thermic influence on the plume. The dependance of wind speed with height is described by the known power law. Emission conditions and transport process is assumed to be constant for one hour. Transport is done with the wind.

Applying this model air pollution concentrations are calculated at any point downwind from a set of sources that may be point,line or even area sources.

Applications of the model

Pollution concentrations are calculated for each possible turbulence situation described by wind speed, wind direction and turbulence class. In connection with recorded frequencies of turbulence conditions a probability distribution of air pollution concentrations is gained. The joint frequency distribution of turbulence conditions should represent a time range of at least five years or more.Examples of calculated probability distributions of the air quality expected are shown in figs. 1 and 2. Figure 1 is typical for the frequency distribution per concentration interval; this figure has already been shown during the fourth meeting of NATO/CCMS at Oberursel in 1973. Figure 2 is a display of the excess frequency distribution of pollution concentrations calculated corresponding to a five years cycle of observed turbulence situations.

The main intention showing these examples is to demonstrate that the statement given by the calculations mostly is of a statistical sense - as Professor Fortak has already mentioned in a previous paper of this meeting -. The calculation of air quality for a single meteorological situation is of much less accuracy than the statistical statement, of course.

Another important point is that calculations cannot be done for situations with wind speeds lower than 1 m/s. For low wind speed situations the turbulent diffusion is comparable in size with the drifting effect in the atmosphere. We therefore have tried to make an estimate of the influence of low wind speed situations relative to all possible turbulence situations on the distribution of concentrations measured. On the basis of concentration measurements at ground level around an industrial plant for about half a year we compared the excess frequency distribution of all measured data with the excess frequency distribution for the measured and calculable data, that means that data corresponding to low wind speed situations have been excluded. Results are given in figs. 3 and 4. The excess frequencies of all measured data shift to somewhat lower values for the measured and calculable data. The conclusion then is made that calculated excess frequency distributions as the one shown in fig. 2 have to be corrected due to low wind speed situations by a factor to be constant in the first approximation. The correction factor was estimated to be about 1.2 or 1.25 comparing the concentration values at an excess frequency of 2,5 %.

At that time we have no further experience if this correction factor is valid for other meteorological or topographical conditions than those in the special region of Cologne or how large the uncertainty of the correction factor will be.

Basic concentration load measurements, however, done within regions of 3 kilometers in diameter indicated that significant values of the concentration distributions derived for all measured data and the same data excluding the low wind speed data differed by about 10 %.

Another application of the model is shown in figs. 5 and 6. The shaded area identifies with an industrial plant that should be expanded by another plant part similar in size as the existing one. The lines represent constant significant values of measured concentrations in mg/m^3. Measurements were done within a region of 5 kilometers in diameter representing the area under investigation. Calculations of the concentrations to be expected due to the emissions of the plant part to be settled were added to the measured concentration data. Fig. 5 shows the mean air quality concentration and fig. 6 the air quality not exceeded for about 97,5 % of time. The drawn lines correspond to the measured basic load. The dotted lines represent the pollution load after the new plant parts have started up operation. A correction due to low wind speed situations like that mentioned before was executed, too. Significant concentration values of the excess frequency distributions have changed by about 10 %, only, in the area of about 2,5 kilometers around the plant though the expansion corresponds to the same plant size as the already existing plant. This relatively small change of pollution load is due to a high basic load of the region at all.

Although the calculated futurous concentration values seem to be low in comparison to the existing basic load calculations will not be too far from reality.

Conclusive remarks

The question of accuracy, of course, is of great importance in all prognostic calculations. Because of the irreversability of the decision in licensing procedures and the degree of uncertainty the handling of the model today includes a security factor of 2. Doing this, decisions have a high probability to be on the safe side. It cannot, however, be taken out of care that using an uncertainty factor of 2 the realisation of industrial settlements or expansions may be questionable because of the deficit of sufficient area.

Reducing this uncertainty factor of 2 to the value of 1 necessary protection distances between industrial and residential areas may be reduced by some hundreds of meters. By this we see the rivality of high security on the one hand and the realisabilty of industrial expansion on the other. What we do need is an optimal solution of the problematic, that is we do need practicable models with a high degree of accuracy.

A realistic way of making decisions will be stating limits for the licensing as follows:

Concentrations to be expected after a plant expansion or a plant settlement should if calculated with this model on the basic of statistical turbulence data

1. never exceed the maximum concentrations admissable to working people,

2. not exceed the limits of concentration load inducing injurious health effects to all people like children,

sick and old people for more than one percent of time over a large period in a statistical sense, i.e. for about 90 hours per year,

3. not exceed the limits of concentration load inducing molestation to all people for more than three or at maximum five percent of time over a longer period, i.e. for about 250 or at maximum 450 hours per year.

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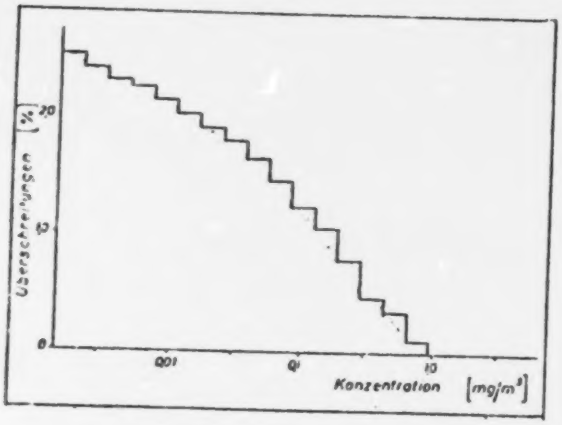

Übergschreitungen [%]
20
10
0
0,01
0,1
10
Konzentration [mg/m³]

Fig. 2

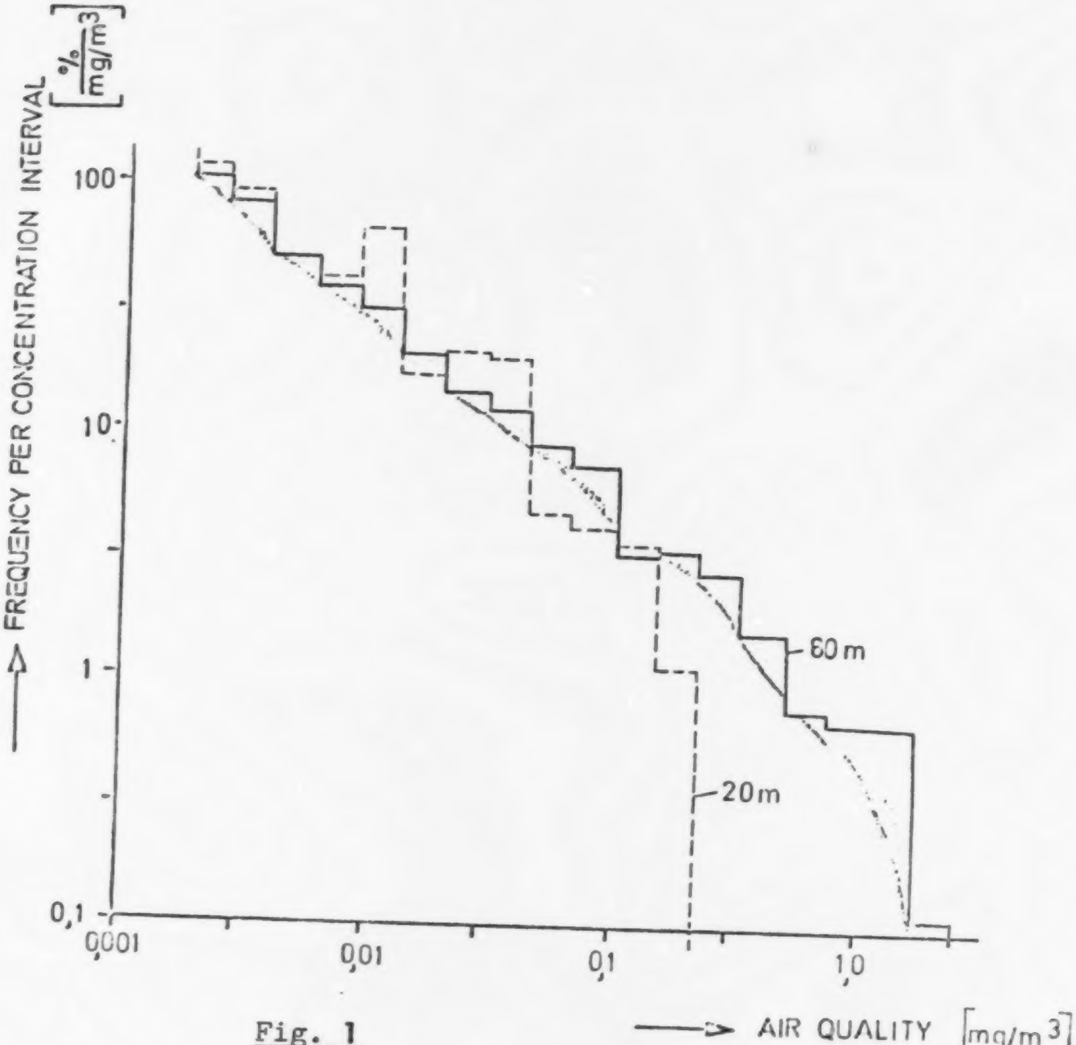
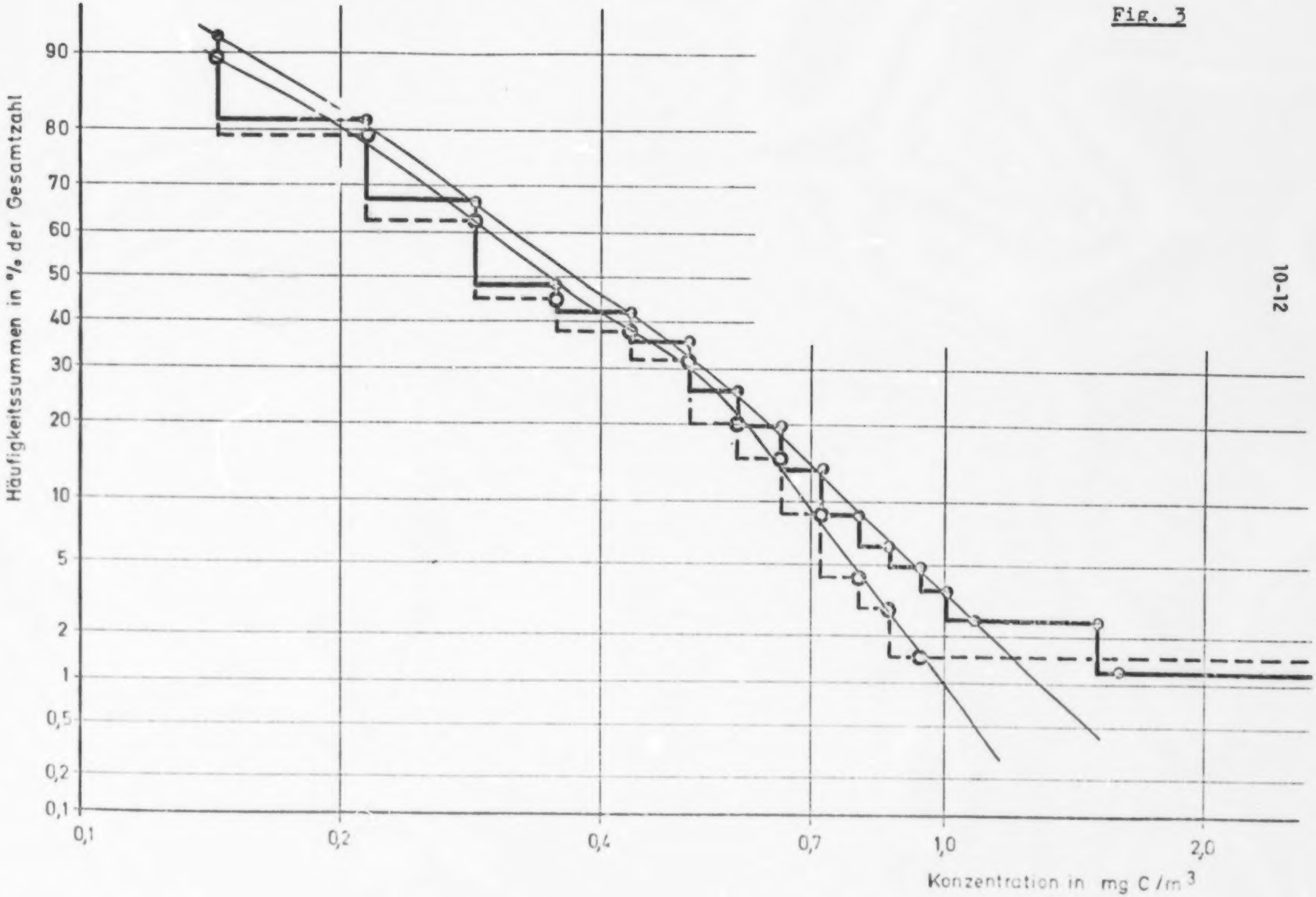

→ FREQUENCY PER CONCENTRATION INTERVAL [%/mg/m³]
100
10
1
0,1
0,001
0,01
0,1
1,0
60 m
20 m
→ AIR QUALITY [mg/m³]

Fig. 1

Fig. 3


Häufigkeitssummen in % der Gesamtzahl
90
80
70
60
50
40
30
20
10
5
2
1
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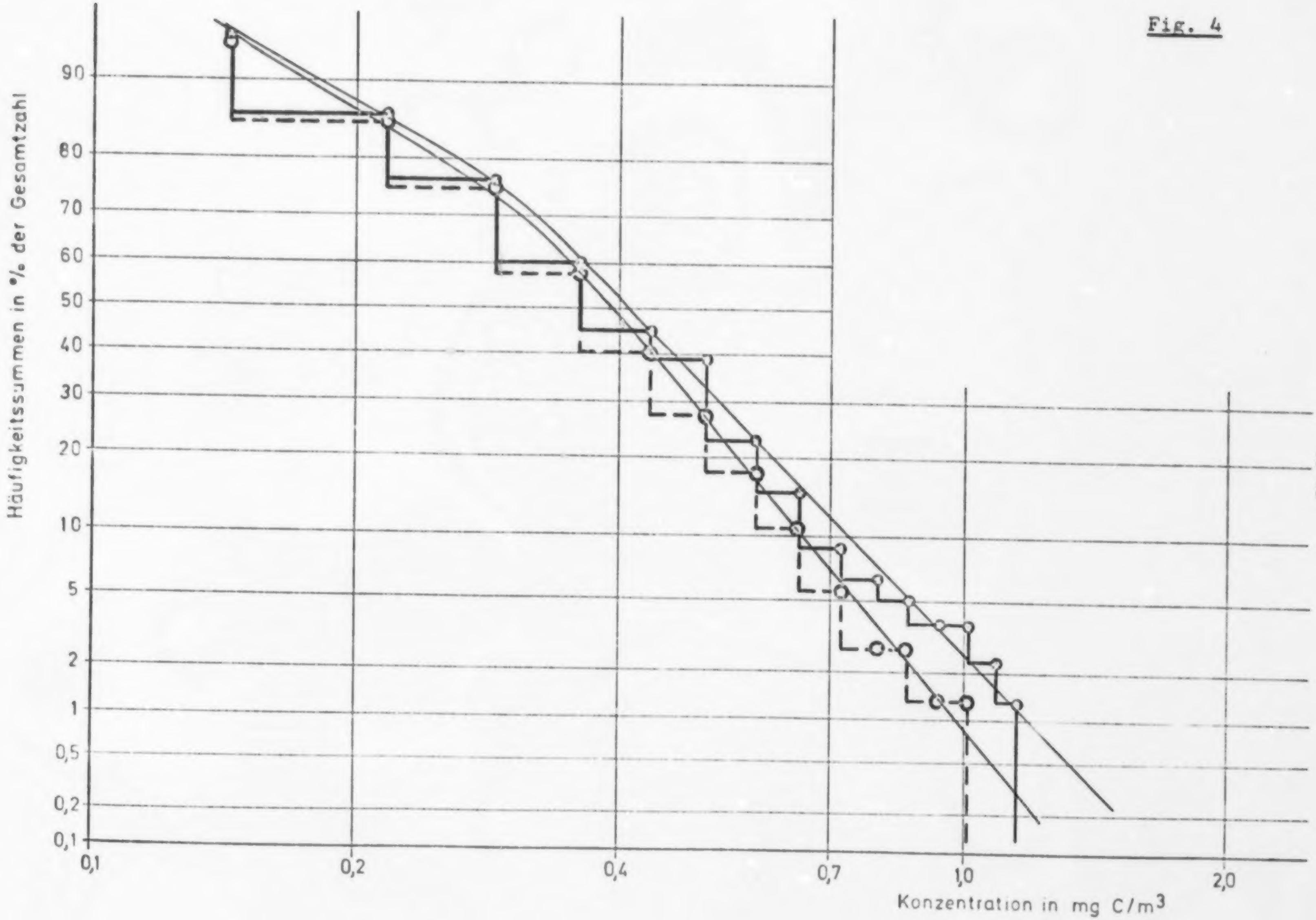
0,2
0,1
0,1
0,2
0,4
0,7
1,0
2,0
Konzentration in mg C/m³

Fig. 4


Häufigkeitssummen in % der Gesamtzahl
90
80
70
60
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0,1
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0,2
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1,0
2,0
Konzentration in mg C/m³

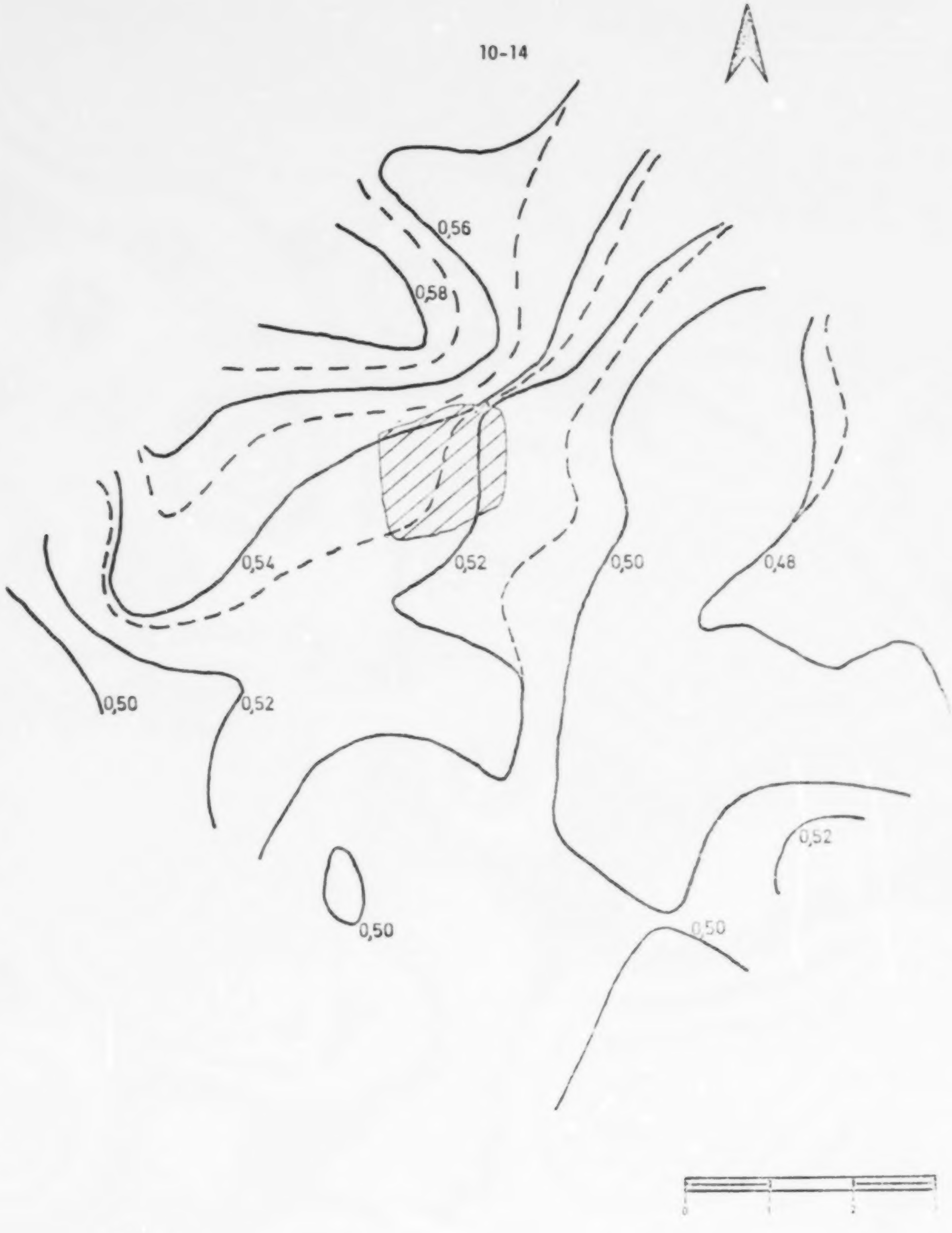
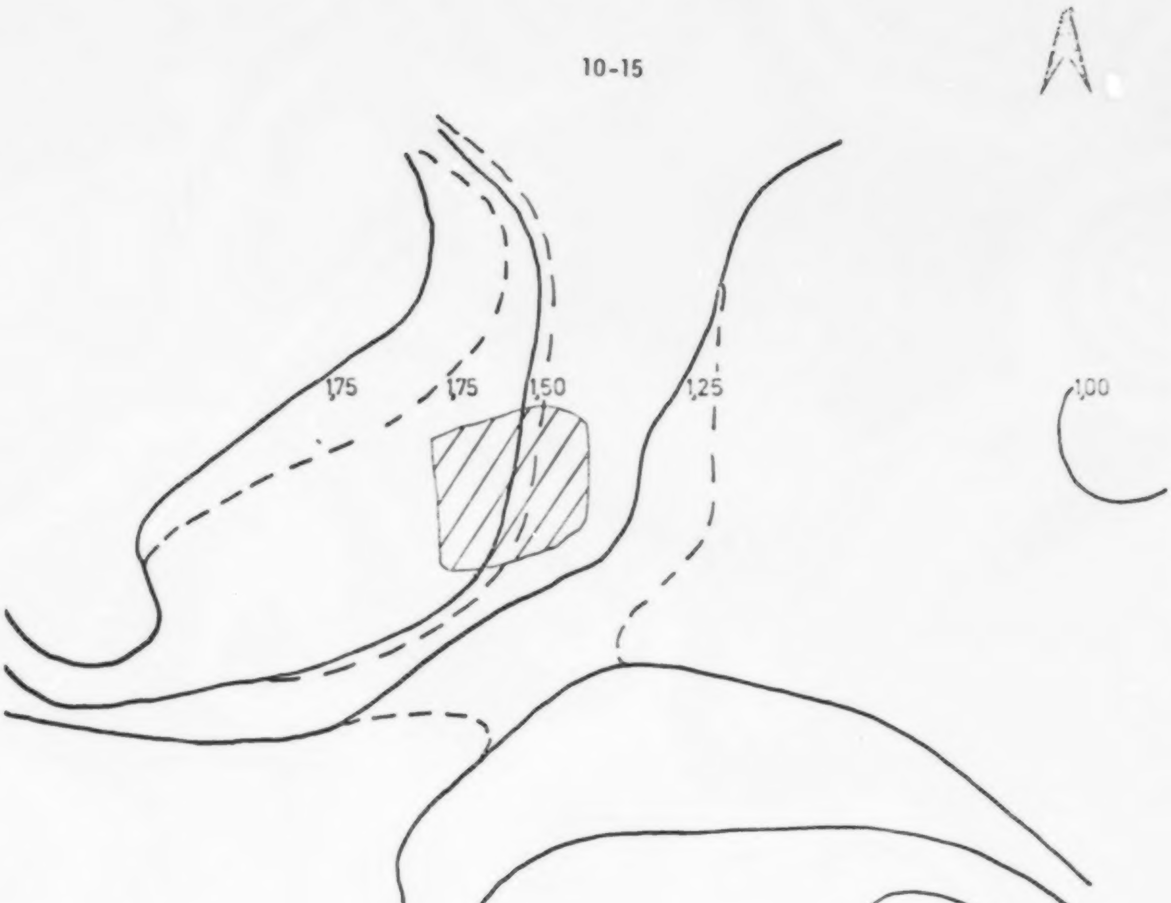

10-14
0,56
0,58
0,54
0,52
0,50
0,48
0,50
0,52
0,52
0,50
0,50
0
1
2
3

Fig. 5



10-15
1,75
1,75
1,50
1,25
1,00
1,25
1,50
1,75
2,00
0
1
2
3 km

Fig. 6

Chapter 11

REQUIREMENTS OF AIR QUALITY MODELS FOR LAND USE PLANNING

by

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[The paper was prepared as part of a NATO/CCMS Fellowship study, while the author was visiting the Meteorology Laboratory, U. S. Environmental Protection Agency]

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REQUIREMENTS OF AIR QUALITY MODELS FOR LAND USE PLANNING

K. E. Grønskei, Norwegian Institute for Air Research

1. Introduction

Air pollution control can be divided into engineering and regulatory control. Engineering control includes all technical devices used to clean flue gases and to prevent emission of pollution. Regulatory control includes the system of all those restrictions and recommendations aimed at reducing ambient air concentration of pollutants. The intention with a regulatory control system is to eliminate or minimize the harmful effects of pollution at the most economical cost for the total society. Generally regulatory control may be divided into Air Quality Management and Land-Use Planning.

Air quality management is responsible for surveillance and control of our air quality, taking the harmful effects of air pollution into consideration. The intention with land-use planning is to plan our physical environment in the best way. Air quality management is a fairly new area of consideration which is being worked into the administrative system, and it should be seen as a part of a comprehensive system aimed to secure, improve and develop our physical environment. Land-use planning is an important area in the development of our society where air quality considerations ought to be included along with other considerations. Land-use planning may take place on several administrative levels and aims to coordinate different kinds of activity. An exchange of experience is now going on between countries within OECD on the use of techniques to provide information necessary to include air pollution considerations in land-use planning (1).

In land-use planning, the following aspects of our society have to be considered: industrial and residential development, recreational and agricultural activity, and aesthetic and environmental considerations. A developed land-use plan will often be a compromise between different competing interests. In the system of considerations that leads to a land-use plan, there exists social, political and environmental constraints, and air quality represents one of the environmental constraints. The intention with this paper is to consider the requirements for air quality information for land-use planning and to consider how these requirements may be formulated in order to be useful in the development or in the selection of existing A.Q. models.

2. Requirement for information to include air pollution considerations in land-use planning

Since air quality considerations have to be compared with many other considerations, they should be presented in a quantified way whenever this is possible. If the air pollution considerations are presented in only a qualitative way, the results may be used to serve special interests in the society. The effects of air pollution may be related to ambient air concentrations. This is very useful information for communication between the political authorities and the air quality control administration. In some countries this communication has resulted in ambient air quality standards. By establishing the connection between emission and ambient air concentrations, regulatory control techniques may be developed.

Different planning methods exist where it is easy to incorporate air pollution considerations. These are methods by which the same amount of emission may be spatially organized in different ways in order to avoid or minimize adverse effects due to air pollution.

a) Location of large stationary sources. Many of the air pollution problems which exist today are caused by industries that are poorly located from an air pollution point of view. This should be avoided by improved planning which, to a large extent, employs studies of local meteorology, climatology and topography in order to improve spatial arrangements for industrial, residential and commercial areas.

b) Location of sensitive receptors. In the planning process, special attention should be given to the old, the sick and to young people. Facilities for their use should be placed in regions with a low pollution level.

c) Small open spaces. Small open spaces around low level sources, for instance around a road with heavy traffic, will improve local dispersion and in that way reduce the ambient air concentration locally. The filtration effect of vegetation should also be considered.

d) Transportation planning. A well planned transportation system can often substantially reduce the pollution concentration.

e) A densely populated region may be organized in different ways, e.g. around one large center, around several smaller centers with open areas in between, in a long corridor or in several corridors pointing out from one center.

These different forms will lead to different ambient air concentrations of pollution due, among other things, to dispersion conditions and total emission from car traffic.

f) Organization of the different utilities within the region to be developed. The spatial arrangement of industrial, commercial and residential areas influence the air quality significantly, for instance by reduction of peak hour traffic in certain residential areas.

Each of these planning methods may influence the future air quality significantly, and models are needed to quantify the difference in air quality as a result of different source distributions. The quantification of ambient air pollution concentrations is dependent on the quantity and conditions of emission, and on the atmospheric dispersion conditions. The different planning methods influence the source distribution on different spatial scales e.g. the large stationary sources often emit most of the pollutants through a stack that may be approximated by a point source. The organization of a densely populated area in different ways influences the source distribution on a regional scale (typical length of several kilometers). The single sources of pollutants are not so important in these considerations and the requirements of A.Q. models are different.

Depending on the adverse effects different statistical parameters of the pollutant concentration may be of importance, e.g. the effects may be dependent on the long-term averaged concentration and/or on the short-term concentrations. Due to the variability in the meteorological processes describing the connection between emissions and ambient air concentration, different requirements may be given to the air quality models depending on the pollutant under consideration and on the climatology of the region where the land-use planning takes place.

To specify the requirements of A.Q. models for land-use planning the following elements have to be considered:

a) The spatial scale of the source distribution to be influenced by the planning method.

b) The statistical parameters of the ambient air concentration that have relevance to the adverse effect.

c) The climatology of the area where the land-use plan is developed.

By considering these three elements, requirements may be specified and relevant assumptions may be made for development and/or application of A.Q. models. It is of primary importance that the parameters determining the differences in air quality that result from different land-use plans are included in the air quality models.

The different planning methods influence the emission distribution on different scales and the following three examples are selected for specification of requirements of A.Q. models:

1) When a location for a large stationary source is to be selected, a quantification of the impact in the form of the distribution of pollution concentration in the surroundings of a single stack is needed.

   Emissions from a single stack may be approximated by a point source. It is well known that under certain meteorological conditions the concentration is approximated well by a Gaussian plume formula.

2) In order to take air quality constraints into consideration in transportation planning, a quantification of changes in the pollution concentration in a street canyon due to changes in the traffic density and to changes in the traffic flow pattern regulated by stop lights is useful.

3) For the organization of a densely populated region, a model to quantify the ambient air concentration on a regional scale due to different emission distributions is needed. The emission distribution may be changed by decisions on zoning, definition of emission factors in different areas, spatial arrangement of the different utilities and transportation planning on a regional scale. Often several different plans are applicable, and a quantification of the difference in air quality between these plans is needed.

The three different applications have been selected to show that different models may be needed on different spatial scales. A simple scale analysis is useful to show this.

In this scale analysis two different classes of meteorological conditions will be considered:

1) The local windfield and turbulence conditions are horizontally homogeneous and determined by large scale air streams.

2) Mesoscale and/or microscale meteorological processes are important to describe the local wind and turbulence conditions.

The first class of meteorological conditions is often observed in the atmosphere especially in flat areas, and important simplifications may be made in the development of A.Q. models.

The second class includes a large spectrum of atmospheric conditions and each of them provides special requirements for A.Q. models. The significance of these requirements have to be determined by considering the points b) and c) on pages 5 and 6.

3. Scale analysis to make simplifications in A.Q. models relevant to the requirements for information.

In the previous section it was specified that the requirements for information from A.Q. models should consider three elements. Three examples of applications of air quality models were selected in order to consider modeling of the impact from air pollution sources with different spatial scales. Two classes of meteorological conditions were selected that may require different air quality models. In order to see how the requirements for information may be used to develop relevant simplifications for the air quality models, a scale analysis will be made of the terms in the general equation describing the connection between emissions and ambient air concentrations. The continuity equation for the pollution component, taking into account sources and sinks of the pollution component, may be formulated in the following way:

$$\frac{\partial c}{\partial t} - u\frac{\partial c}{\partial x} - v\frac{\partial c}{\partial y} - w\frac{\partial c}{\partial z} - \frac{\partial T_x}{\partial x} - \frac{\partial T_y}{\partial y} - \frac{\partial T_z}{\partial z} + Q + R \qquad (1)$$

t = time coordinate

x,y,z = the coordinates in a rectangular coordinate system

c = pollution concentration

u,v,w = the wind components along the x,y,z axes respectively

T_x,T_y,T_z = the turbulent transport of pollutants

Q = volume sources of pollution

R = reaction rate

Typical non-dimensional (primed) values of the different parameters are defined by:

$$c = \bar{c}\,c', \quad u = \bar{u}\,u', \quad v = \bar{v}\,v', \quad w = \bar{w}\,w'$$

$$T_x = \bar{T}_x\,T_x', \quad T_y = \bar{T}_y\,T_y', \quad T_z = \bar{T}_z\,T_z'$$

$$Q = \bar{Q}\,Q', \quad R = \bar{R}\,R'$$

$$t = \bar{t}\,t', \quad x = \bar{x}\,x', \quad y = \bar{y}\,y', \quad z = \bar{z}\,z'$$

$$\left.\begin{array}{l}\bar{c}\\ \bar{u}\\ \bar{v}\\ \bar{w}\\ \bar{T}_x\\ \bar{T}_y\\ \bar{T}_z\\ \bar{Q}\\ \bar{R}\end{array}\right\}$$

The characteristic values of the variables describing the situation are defined so that the corresponding primed, nondimensional values vary between zero and one within the area under consideration.

$$\left.\begin{array}{l}\bar{t}\\ \bar{x}\\ \bar{y}\\ \bar{z}\end{array}\right\}$$

The characteristic values of time, and the horizontal and vertical scales of the problem are defined so that the derivatives of the ambient air concentrations and of the turbulent fluxes of pollutants vary between zero and one within the area under consideration.

By using these typical nondimensional values Equation (1) may be written:

$$\frac{1}{\bar{t}}\frac{\partial c'}{\partial t'} = -\frac{\bar{u}}{\bar{x}}u'\frac{\partial c'}{\partial x'} - \frac{\bar{v}}{\bar{y}}v'\frac{\partial c'}{\partial y'} - \frac{\bar{w}}{\bar{z}}w'\frac{\partial c'}{\partial z'}$$

$$-\frac{\bar{T}_x}{\bar{x}\,\bar{c}}\frac{\partial T_x'}{\partial x'} - \frac{\bar{T}_y}{\bar{y}\,\bar{c}}\frac{\partial T_y'}{\partial y'} - \frac{\bar{T}_z}{\bar{z}\,\bar{c}}\frac{\partial T_z'}{\partial z'} + \frac{\bar{Q}}{\bar{c}}Q' + \frac{\bar{R}}{\bar{c}}R' \qquad (2)$$

In order to compare the magnitude of the different terms in Equation (2), the following numbers may be compared:

$\frac{1}{\bar{t}}$: the time variation of the pollution concentration.

$\frac{\bar{u}}{\bar{x}}$; $\frac{\bar{v}}{\bar{y}}$; $\frac{\bar{w}}{\bar{z}}$ } The magnitude of the horizontal and vertical advection terms.

$\frac{\bar{T}_x}{\bar{x}\,\bar{c}}$; $\frac{\bar{T}_y}{\bar{y}\,\bar{c}}$; $\frac{\bar{T}_z}{\bar{z}\,\bar{c}}$ } The magnitude of the horizontal and vertical turbulent transport terms.

$\frac{\bar{Q}}{\bar{c}}$; $\frac{\bar{R}}{\bar{c}}$: The magnitude of the sources and sinks of the pollution component.

The typical values for the turbulent fluxes are often estimated to be proportional to the gradient in the pollution component:

$$T_x = K_x \frac{\partial c}{\partial x} \;;\; T_y = K_y \frac{\partial c}{\partial y} \;;\; T_z = K_z \frac{\partial c}{\partial z}$$

The magnitudes of the turbulent transport terms are:

$$\frac{\bar{T}_x}{\bar{x}\;\bar{c}} = \frac{\bar{K}_x}{\bar{x}^2} \qquad \frac{\bar{T}_y}{\bar{y}\;\bar{c}} = \frac{\bar{K}_y}{\bar{y}^2} \qquad \frac{\bar{T}_z}{\bar{z}\;\bar{c}} = \frac{\bar{K}_z}{\bar{z}^2}$$

The two meteorological situations to be considered are specified as follows:

1) The situations are characterized by stationary and homogeneous wind and turbulence conditions determined by large scale air streams. The temperature stratification is assumed to be neutral. The x-axes of the coordinate system is oriented along the mean air stream.

2) The situation is characterized by low horizontal advection velocity. The wind may be inhomogeneous and the temperature stratification is stable (inversion) suppressing vertical turbulent transport.

A) A.Q. model for a quantification of the pollution concentration in the surroundings of a single stack.

The spatial scales $(\bar{x}, \bar{y}, \bar{z})$ as they are defined above vary substantially with the distance from the stack. In the atmosphere turbulence elements are present on all spatial scales. Elements with spatial scales that move the whole plume close to the stack may act effectively to dilute the plume further away from the stack. Empirical evidence shows that a Gaussian plume formula describes well an ensemble mean value of the concentration distribution in the surroundings of the stack.

From a theoretical point of view a Gaussian plume formula may be found as a solution of the equation:

$$u \frac{\partial c}{\partial x} = K_y \frac{\partial^2 c}{\partial y^2} + K_z \frac{\partial^2 c}{\partial z^2} \qquad (3)$$

Formulated by typical mean values this means that the numbers $\frac{\bar{u}}{\bar{x}}$ and $\frac{\bar{K}_y}{\bar{y}^2}$ and $\frac{\bar{K}_z}{\bar{z}^2}$ have to be at least one order of magnitude larger than the other numbers expressing the magnitude of the other terms in Equation 2. These requirements are fulfilled in weather conditions belonging to the class of meteorological situations characterized by homogeneous wind and turbulence conditions. When inhomogeneous wind and turbulence conditions occur, for example due to topography $\left(\frac{\bar{v}}{\bar{y}} \approx \frac{\bar{u}}{\bar{x}} \text{ or } \frac{\bar{w}}{\bar{y}} \approx \frac{\bar{u}}{\bar{x}} \right)$, special considerations have to be made to quantify the ambient air concentration due to a single stack.

B) A.Q. model for a quantification of the pollution concentration in a street canyon.

The cars moving along a street emit pollutants. A typical spatial scale along the street $(\bar{x})$ becomes very large, and the line of moving cars may be considered as a line source. It is the transport and diffusion perpendicular to the line source that are important for the ventilation. If mean concentrations within a street canyon are considered, the width of the street and the height of the houses may be used to describe the spatial scales perpendicular to the street canyon $(\bar{y},\bar{z})$. The air streams within the street canyons are very complex, and the ventilation may be described by a diffusion and/or by a transport process. The street canyon submodel developed by W. Johnson et al., at Stanford Research Institute assumes that the flux out of the street canyon is proportional to the locally generated CO emissions in the street, and that a helical circulation (primary vortex) in the street canyon cause the main ventilation (2).

It is difficult to quantify the characteristic values of the variables describing the emission-ventilation conditions. Large variations are likely to be observed with time. To estimate the effectiveness of the ventilation in relation to the emissions, continuous measurements of the CO concentrations were made. The emissions fluctuated in time in accordance with the traffic density controlled by a traffic stop light. From the response in the ambient air concentration in the street canyon, an indication of the typical ventilation parameters is given:

$$\frac{1}{\tau} = \max \left\{ \frac{\bar{v}}{\bar{y}} \; ; \; \frac{\bar{w}}{\bar{z}} \; ; \; \frac{K_y}{\bar{y}^2} \; ; \; \frac{K_z}{\bar{z}^2} \right\}$$

In a street in Drammen, Norway, it was found that:

On September 12, 1972 $\tau = 42$ s

On October 6, 1972 $\tau = 41$ s

A detailed description of the procedure used to find these values is given in Appendix 1.

In order to study the variations in the pollution conditions with meteorological parameters, traffic conditions, etc. some measurements of the variation in pollution concentration within this time scale should be made. The spatial scales involved are assumed to be equal to the width of the street ($\bar{y}$ = 30m) and to the height of the houses ($\bar{z}$ = 10m). Measurements used to develop further a street canyon air quality model should resolve the following variations of the parameters.

$$\bar{v} = \frac{\bar{y}}{\tau} \qquad \bar{v} = \frac{30\text{m}}{40\text{s}} = 3/4 \ \text{m/s}$$

$$\bar{w} = \frac{\bar{z}}{\tau} \qquad \bar{w} = \frac{10\text{m}}{40\text{s}} = 1/4 \ \text{m/s}$$

$$\bar{K}_y = \frac{\bar{y}^2}{\tau} \qquad \bar{K}_y = \frac{900\text{m}^2}{40\text{s}} = 90/4 \ \text{m}^2/\text{s}$$

$$\bar{K}_z = \frac{\bar{z}^2}{\tau} \qquad \bar{K}_z = \frac{100\text{m}^2}{40\text{s}} = 10/4 \ \text{m}^2/\text{s}$$

If variations with these amplitudes are resolved, the variations that are important for the fluctuations in the ambient air concentration will probably be detected.

C) A.Q. models to quantify air pollution concentration on a regional scale.

For the organization of a densely populated region a model to quantify the ambient air concentration on a regional scale due to different emission distributions is needed. The source distribution is influenced on a horizontal scale $\pm$ a few kilometers ($\bar{x}$ and $\bar{y} \approx 5.10^3$ m). The vertical scale is of the order of 100 m ($\bar{z} \approx 1.10^2$ m).

To see how different models may be needed in different meteorological situations, the wind and turbulence conditions are specified in the following way:

1. When the wind and turbulence conditions are homogeneous and the temperature stratification is neutral, the wind and turbulence conditions are specified by:

$$\bar{u} = 5 \text{ m/s} \quad ; \quad \bar{K}_z = 5 \text{ m}^2/\text{s}$$

2. When the windspeed $|\bar{v}|$ is low ($|\bar{v}| \approx 1$ m/s) and the temperature stratification is stable ($K_z \approx 0.2$ m^2/s), the wind direction is often inhomogeneous.

Where the horizontal windfield is inhomogeneous, the horizontally convergent and/or divergent part will cause vertical motions. It is assumed that the vertical velocity may be found directly from the horizontal divergence and that the vertical velocity is zero at the ground.

$$W_H = -\int_0^H \left(\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) dz$$

During some case studies in Oslo the convergence towards the city center was found to be in the order of $10^{-4} - 10^{-3}$ s^{-1}. (3) Some case studies from St. Louis have also shown convergent air streams close to the ground over the urban area. Convergence values up to 10^{-4} s^{-1} have been observed (4).

The horizontal eddy diffusion:

The eddy diffusion coefficients (K_x,K_y) are, among other things, dependent on the decomposition of the wind field into an average component and a turbulent component. If a finite difference approximation of the continuity equation is selected for the model development, a certain spatial resolution of the wind field is chosen. The diffusivity of eddies with a spatial scale larger than 2-4 times the grid distance should be described by the time variation of the wind field specified in the grid system. This turbulent effect may in principle be described as a stochastic part superimposed on the mean wind field.

The diffusive effect of eddies with a spatial scale smaller than the grid elements has to be estimated. The K-theory may be used when the spatial scale of the diffusive turbulent elements is restricted in this way. On the other hand the problem is then transferred to a realistic description of the stochastic wind component. In order to compare the different terms in the continuity equation the grid distance is assumed to be 1,000m, and the horizontal diffusion coefficient is assumed to be $K_x = K_y = K_h = 100\ m^2/s$.

The emission of pollutants

This term represents the forcing term in the modified continuity equation. If the magnitude of this term is known, the magnitude of some other terms has to be of the same order of magnitude. To estimate a typical emission from low level sources in an urban area, data from Oslo on the SO_2 emission (3) are used.

The mean emission rate from an area of about $50km^2$ over the center of the city is used to estimate a typical emission value. The height of the volume source is assumed to be 100 m. Based on these assumptions a typical value of the volume source ($\bar{Q}$) is found to be:

$$\bar{Q} \approx 1\ \mu g\ SO_2/\ m^3 s$$

As a summary, Table I specifies the magnitude of the different terms in Equation 2 connected to the meteorological situation.

TABLE I

A quantification of the different terms in the modified continuity equation (Equation 2). Unit: s^{-1}

	advection		diffusion	
	$\frac{\bar{u}}{\bar{x}}$; $\frac{\bar{v}}{\bar{y}}$	$\frac{\bar{w}}{\bar{z}}$	$\frac{\bar{K}_x}{\bar{x}^2}$; $\frac{\bar{K}_y}{\bar{y}^2}$	$\frac{\bar{K}_z}{\bar{z}^2}$
homogeneous advection diffusion situation	10^{-3}	Zero	$4 \cdot 10^{-6}$	$0.5 \cdot 10^{-3}$
stagnant inversion situation	$2 \cdot 10^{-4}$	10^{-4}	$4 \cdot 10^{-6}$	$2 \cdot 10^{-5}$

The numbers show the relative importance of the horizontal and vertical ventilation terms in an air quality model to be used for land-use planning on a regional scale. In a meteorological situation with homogeneous advection and turbulence,the vertical transport and the horizontal diffusion are small. The numbers describing a stagnant inversion situation, show that a small horizontal velocity (1 m/s) may have an important effect on the ventilation. Empirical observations indicate that systematic vertical motion over an urban area is important. The horizontal diffusion is not important for the description on a regional scale. The vertical turbulent transport may be of importance even in inversion situations. After a time (comparable to the inverse value of the numbers in TABLE I) the ambient air concentration will approach a steady state where the ventilation is equal to the source strength.

Regarding the sinks of air pollution due to chemical reactions, these become important when the inverse value of the typical reaction time is comparable with the numbers in TABLE I. A chemical reaction with a reaction time of a few hours is not very important in situations with advection, but becomes important in stagnant inversion situations.

4. Concluding remarks

It has been identified that in order to specify requirements to be useful in selection and/or development of A.Q. models, three elements have to be considered:

a) The different land-use planning methods influence the source distribution on different spatial scales and information on air quality is therefore required with different spatial resolutions. This information may be used to develop simplifications for A.Q. models, specifically if the conditions in inhomogeneous meteorological situations have to be described.

b) The statistical parameters describing the ambient air concentrations that are important for the adverse effects, have to be determined for the different pollutants. Often it is the annual mean concentrations that are considered in relation to land-use planning. If peak concentrations are important, in relation to the adverse effects, a model is needed for the stagnant meteorological conditions when the ambient air concentration is ten times higher than in situations with generally higher advections.

c) The climatology of the area has to be considered in order to determine the frequency and types of meteorological situations in the area where the plan is going to be developed. The frequency of the adverse meteorological situations may be high enough to influence the seasonal mean value. In this way different A.Q. models may be needed depending on the pollutant component and on the climatology in the area under consideration. When the wind and turbulence conditions are homogeneous, models based on the Gaussian plume formula represent a powerful tool to quantify the air pollution impact due to land-use planning on different spatial scales. These models apply under specific meteorological situations. The need for other types of A.Q. models is dependent on:

1. The adverse effects of the pollution under consideration.
2. The frequency of situations with nonhomogeneous wind and turbulence conditions and the pollution concentration in these situations.

The requirements of A.Q. models are highly dependent on the formulation of the constraints and on the expected air quality. If good air quality is expected in an area (few sources), the air quality considerations will not be given much weight in the planning decision process. However, if a poor air quality is expected, i.e. the forecasted ambient air concentrations exceeds air quality standards, the air quality considerations are of decisive importance. The importance of taking air quality into consideration on the planning stage is underlined by the fact that it is very difficult and expensive to correct mistakes once a plan has been developed.

Acknowledgements

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Appendix 1: A method to determine the typical ventilation time for a street in Drammen, Norway.

A continuous monitoring station for CO (UNOR - 2) was placed downstream (with respect to traffic) of a traffic light in a street in Drammen, Norway. All cars moved in the same direction. The cars had to pass an open space before entering the street canyon where the measuring instrument was placed. The cars arrived in groups determined by the green light period from the traffic stop light. The observed response in the ambient air concentration from two case studies is shown in Figure 1 and 2.

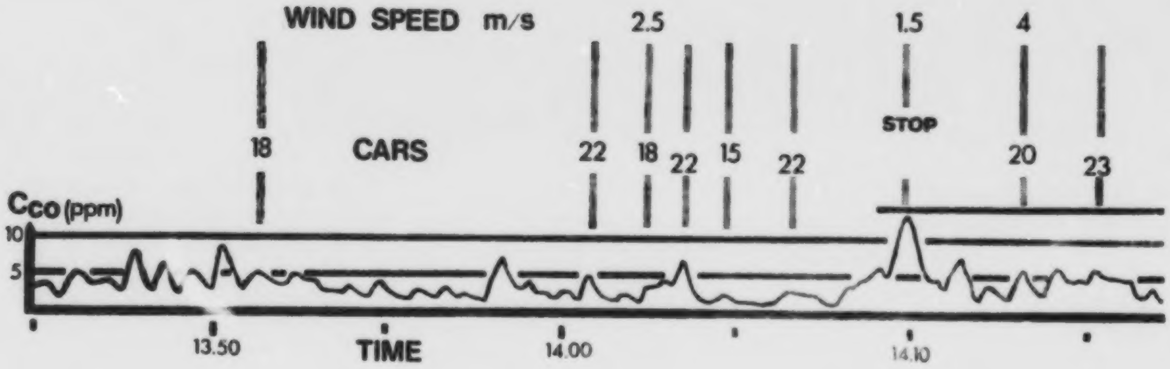

Figure 1: CO-concentration downstream of a stop light in the city of Drammen, Sept. 12, 1972.

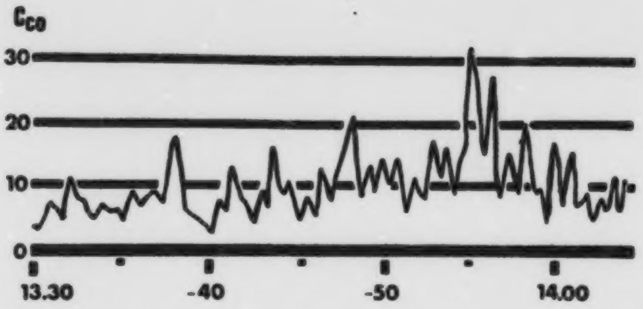

Figure 2: CO-concentration downstream of a stop light in the city of Drammen, Oct. 6, 1972.

A period of 55 seconds, corresponding to the frequency of the stop light is easily identified. The fluctuations take place above a lower concentration, and a large variation in the amplitude is observed mostly due to differences in the ventilation.

If the ventilation is assumed to be proportional to the concentration, the equation describing the nonstationary process may be formulated in the following way:

$$\frac{\partial c(t)}{\partial t} = - \frac{c(t)}{\tau} + Q(t) \qquad \text{(A.1)}$$

$c(t)$: concentration of CO

τ : typical ventilation time

$Q(t)$: volume source of pollutant

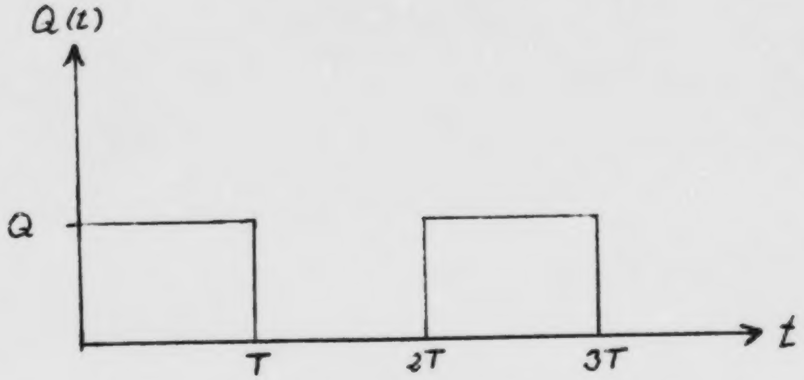

Figure 3: The emission variation with time.

It is assumed that the volume source has a variation with time presented in Figure 3. The initial conditions are specified by:

$$C\ (0) = C_0 \tag{A.2}$$

The solution of Equation A.1, given the specified emission distribution with time and the initial conditions specified in Equation A.2:

$$\begin{aligned} C(t) &= (Q\,\tau\,(1-e^{-t/\tau}) + C_0\ e^{-t/\tau})\ , \quad 0 \le t < T \\ C(t) &= (Q\,\tau\,(1-e^{-T/\tau}) + C_0\ e^{-T/\tau})\ e^{-(t-T)/\tau}, \quad T \le t < 2T \end{aligned} \tag{A.3}$$

Defining δ as the difference in ambient air concentration over a time period (2T) determined by the frequence of the stop light, δ, is specified in equation (A.4).

Equation (A.3) is used to determine δ_1:

$$\delta_1 = C(2T) - C(0)$$

$$= (Q\tau + (C_o - Q\tau)\ e^{-T/\tau})\ e^{-T/\tau} - C_o \qquad (A.4)$$

Two dimensionless variables are defined:

$$X \overset{def}{=} \frac{T}{\tau}$$

$$A \overset{def}{=} \frac{TQ}{C_o} \qquad (A.5)$$

$$\frac{\delta_1}{C_o} = A\left(\frac{e^{-x} - e^{-2x}}{x}\right) + e^{-2x} - 1 \qquad (A.6)$$

If it is assumed that no accumulation takes place from one period to another, $\delta_1 = 0$.

$$A = \frac{(e^{x} - e^{-x})x}{1 - e^{-x}} \qquad (A.7)$$

The amplitude of the fluctuation in the ambient air concentration (Δ) due to the variation in the emission is determined using Equation (A.3).

$$\Delta = C(T) - C_o = Q\tau(1 - e^{-T/\tau}) + C_o\ e^{-T/\tau} - C_o \qquad (A.9)$$

$$\frac{\Delta}{C_o} = A\,\frac{1 - e^{-x}}{x} + e^{-x} - 1$$

A is determined using Equation (A.7):

$$\frac{\Delta}{C_o} = e^{x} - 1$$

$$\tau = T/\ln\left(1 + \frac{\Delta}{C_o}\right) \tag{A.9}$$

The registration of the carbon monoxide concentration shown in Figures 1 and 2 are used to estimate the mean amplitude of the fluctuations in the ambient air concentrations. The ventilation time (τ) is estimated from (A.9).

$\bar{C}\ ((2n + 1)T)$: The mean value of all maximum concentrations occurring with a period of 2T.

$\bar{C}\ (2nT)$: The mean value of all minimum concentrations occurring with a period of 2T.

On September 12, 1972: $2T = 55$ s

$\bar{C}\ ((2n + 1)T) = 5.2$ ppm CO

$\bar{C}\ (2nT) = 2.7$ ppm CO

$\bar{\Delta} = \bar{C}\ ((2n + 1)T) - \bar{C}\ (2nT) = 2.5$ ppm CO

$\dfrac{\bar{\Delta}}{\bar{C}(2nT)} = 0.92$; $\underline{\tau = 42 \text{ s}}$

On October 6, 1972: $2T = 55$ s

$\bar{C}((2n + 1)T) = 13.2$ ppm

$\bar{\Delta} = 6.4$ ppm

$\bar{C}(2nT) = 6.8$ ppm

$\frac{\bar{\Delta}}{\bar{C}(2nT)} = 0.94$

$\underline{\tau = 41 \text{ s}}$

Chapter 12

MODIFIED ROLLBACK MODELS

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskile, Denmark
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MODIFIED ROLLBACK MODELS

by

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Air Quality Models

The concentration of a pollutant in the ambient air varies in both space and time. The spatial-temporal air quality distribution is influenced by the rate, height, spatial, and temporal distribution of emissions as well as the meteorological and topographical conditions in the region of interest. The ideal model for estimating the change in future air quality due to alternative emission control actions would include quantitative considerations of these factors plus atmospheric reaction and pollution-decay processes.

No existing model can handle all of these factors simultaneously. The more advanced "diffusion" models allow some of these factors as inputs, but such models are data hungry. They require large quantities of air quality, meteorological, and emission data for calibration and operation. Until the theory, data, expertise, and model availability improve, simplified models must be used to compare alternative control strategies.

The simplest and most familiar air quality model is the proportional model. This model deals only with the relationship between emissions and concentrations. It is based on the assumption that an indicator of man-made pollutant concentration is directly proportional to man-made emission in the area of interest. Symbolically,

$$\frac{\chi_j - B}{\chi_o - B} = \frac{Q_j}{Q_o} \tag{1}$$

where χ_o = Concentration indicator in the ${}_j$th year

χ_o = Concentration indicator in the base year

Q_j = Total emission in the ${}_j$th year

Q_o = Total emission in the base year

B = Background concentration

This model is a valid, first order approximation of reality if the following set of assumptions are supportable:

1. The indicator of air quality is representative of the air quality distribution over the region of interest.

2. The distribution of emissions in space and time is relatively stable over the projection period.

3. The meteorological and topographical characteristics of the area are stable over the projection period.

4. Average background concentration remains constant over the projection period.

Assumptions 2, 3, and 4 are usually reasonable when analyzing existing urbanized areas. They are not reasonable for new towns or rapidly expanding small towns. Nor are they reasonable when large point sources are added to existing urban areas, for the emission distribution is grossly altered under such circumstances.

The most problematical assumption is Number 1. Air quality is measured by point monitors. Air quality data thus collected provides a good *temporal* profile but is not a good indicator of *areal* distribution of pollution concentration. A point monitor reading may be highly influenced by emissions in its immediate vicinity thereby inaccurately estimating the general air quality over the area of interest. Also, monitors may not be located at the point of maximum regional concentration (see Figure 1). Therefore, the proportional model should not be expected to accurately predict the change of concentration at each and every monitor, but it can be used to estimate the change in average air quality over the urbanized area due to emission changes which are distributed over that area.

The Simple Rollback Model

Emissions may increase due to the growth of urban activities, decrease due to per-source emission limitations, or be affected by a combination of these factors. The *simple* proportional model expresses these factors thus:

$$\frac{X_j - B}{X_o - B} = \frac{Q_j}{Q_o} = \frac{Q_o F_j G_j}{Q_o} = F_j G_j \qquad (2)$$

where F_j = Emission factor ratio

G_j = Growth factor

The emission factor ratio, F_j, is the ratio between the average emission factor for the composite urban source expected in year ($_j$) and that during the base year ($_o$). The growth factor, G_j, is the ratio between the average level of activity in year $_j$ to that during the base year $_o$. (Activity may be measured by the population of people, cars, factories or by vehicle miles traveled, kilowatts generated, etc.)

The simple proportional model is often rearranged by defining a required reduction, R, as:

$$R \equiv (1 - F_j)\ 100\% \tag{3}$$

$$R = \left(1 - \frac{x_j - B}{G_j(x_o - B)}\right)\ 100\% \ = \frac{G_j\ (x_o - B) - x_j + B}{G_j(x_o - B)}\ 100\%$$

$$R \simeq \frac{G_j x_o - x_j}{G_j x_o - B}\ 100\% \tag{4}$$

Equation (4) is the simple "rollback" equation. It estimates the percent reduction in the average per-source emission rate needed in order to attain a pollutant concentration of x_j (usually an air quality standard) given x_j, G_j, and B. Note that both G_j and R are average values. There are several source categories for any pollutant. Each may have a unique emission factor ratio and growth factor. Unless this fact is recognized explicitly, serious errors may be inadvertently made. For example, suppose there are two source categories which emit pollutant X. One source emits 90 percent and the other emits 10 percent during the base year. Suppose also that the dominant source category is growing at 2 percent per year and the lesser source category is growing at 4 percent per year. Finally, assume that present concentration of pollutant X is three times the desired level, B is 1/10 the desired level, and the desired level is to be attained in 10 years.

One approach is to neglect the lesser source category as insignificant. The growth factor would then be calculated from the dominant source growth rate by

$$G_1 = (1 + .02)^{10} = 1.22$$

The simple rollback formula then yields

$$R = \frac{1.22 \times 3 - 1}{1.22 \times 3 - 0.1}\ 100\% = 73\%$$

The proper approach is to include both source categories. The lesser category growth factor is

$$G_2 = (1 + .04)^{10} = 1.48$$

The total emission in year (j) is

$$Q_j = Q_{01}\ G_1F_1 + Q_{02}G_2F_2$$

If the lesser source category is not controlled, then $F_2 = 1.0$ and

$$Q_j = 0.9 \times 1.22 \times F_1 + 0.1 \times 1.48 \times 1.0 = 1.1\ F_1 + .15$$

Inserting this value for Q_j in the proportional formula, we get

$$\frac{1 - 0.1}{3 - 0.1} = \frac{1.1\ F_1 + .15}{1}$$

$$F_1 = .146$$

$$R_1 = (1 - .146)\ 100\% = 85\%$$

So the amount of emission control which must be applied to the dominant source category in order to achieve the desired air quality in 10 years is actually 85 percent rather than the 73 percent estimated by neglecting the lesser source category.

Another advantage of explicitly including all source categories in the calculation of future emission is that this allows the examination of alternative levels of control on different source categories. For the example:

$$\frac{1 - 0.1}{3 - 0.1} = \frac{1.1 F_1 + .15 F_2}{1}$$

$$F_1 = .283 - .136 F_2$$

Values of F_1 and F_2 satisfying this equation are listed below:

F_1	R_1	F_2	R_2
.28	72%	0	100%
.25	75%	.24	76%
.20	80%	.61	39%
.15	85%	1.0	0%

The Modified Rollback Model

The value of explicit consideration of all source categories has led to the development of the "modified rollback" model. The "modification" is simply a disaggregation of the Q_j term of the simple rollback model to reflect the several factors involved in the computation of future emissions. The expanded proportional model is written:

$$\frac{X_j - B}{X_o - B} = \frac{\sum_{i=1}^{n} Q_i G_{ij} F_{ij} K_i T_{ij}}{\sum_{i=1}^{n} Q_i K_i} \qquad (5)$$

Equation (5) may appear a bit formidable. However, it is merely a symbolic representation of the disaggregation of the total emissions of a pollutant and their impact on an area's air quality. Instead of applying growth and control factors to the sum total of the emissions, the disaggregation procedure allows the growth and control factors to be applied separately to emissions from several or many categories of sources. A projected emission total from each category is calculated. The projected emissions from each of the categories are then summed to provide the total emissions used in the simple rollback formulation. This procedure allows the analyst to account for different rates of growth of various segments of the economy and different degrees of control to various sources of pollutants. For example, consider the problem of estimating future total emissions of carbon monoxide on a city. The emissions can be disaggregated into several categories of sources, such as automobiles, trucks, railroads, aircraft, space heating, power generation, refineries, etc. It is improbable that each of these sources will grow at the same rate; nor will controls applied to the different source categories be equally effective. To be specific, in the United States a 1975 model automobile will emit 10 percent of the CO that a 1970 model automobile emits. Yet, the CO emitted by a home heating unit is unlikely to change.

Returning to the equation, the terms on the left side of the equality have previously been defined. The indix i refers to source categories (automobiles, power plants, trucks, etc.). There are n such categories.

The index j refers to the year for which the emissions are projected. The symbol G is the growth rate. The symbol F is the emission factor ratio. Both have been defined earlier.

Two new symbols, K_i and T_{ij} are introduced. K_i is an emission weighing factor. It is introduced to account for the fact that emissions from the several sources may vary in their impact on air quality due to emission height, location, or chemical composition. T_{ij} is a transportation control factor. It allows for the inclusion of emission reduction due to one or combination of transportation controls which are difficult to express in terms of growth or per-source emission factor reduction. However, transportation control effects should be reflected in G_{ij} and/or F_{ij}, if possible.

The emission weighing factor was originally included for use in modeling sulfur dioxide and total suspended particulate matter. Both of these pollutants are often emitted from tall stacks with a consequent diminution of impact on ground-level concentration. However, the Environmental Protection Agency is revising the regulations which specify procedures for evaluating State Implementation Plans to require use of a diffusion model for these pollutants. The use of weighing factors for the height or location of nitrogen dioxide and oxidants is inappropriate due to time delay in the photochemical formation of these pollutants from oxides of nitrogen and non-methane hydrocarbons, their precursors. The weighing factor may be used to characterize the relative reactivities of the various hydrocarbon species.

Carbon monoxide contamination is due almost entirely to mobile sources, and the contribution of stationary sources is heavily discounted in the special CO model to be presented later on. Therefore, the K_i is set equal to 1.0 unless very good reasons for doing otherwise can be presented.

If K_i is set equal to 1.0 for all categories, then the right side of the equation may be rearranged by dividing each term in the numerator by ΣQ_i (total base year emission) and multiplying numerator and denominator by 100 percent. The result is

$$\frac{X_j - B}{X_o - B} = \frac{\sum_{i=1}^{n} P_i G_{ij} F_{ij} T_{ij}}{100\%} \qquad (6)$$

Where P_i is the percent contribution of emission from category i to total emission during the base year.

Application, Limitations, and Alternate Forms of the Modified Proportional Model

The "modified" model is actually an expanded method of computing future emissions which allows flexibility in comparing the effects of alternative emission and growth limitations.

There is no question that urban emissions affect urban air quality. There is considerable question about the linearity of the relationship and about the appropriateness of using one or a few point monitor readings to represent "urban air quality." Therefore, the model presented should be viewed in two parts. The first part is an accurate method of estimating future emissions for the changes in emissions expected due to growth and various control actions. The second part is a first approximation of the relationship between emissions and air quality (represented by the equals sign) and a first approximation of the regional air quality distribution (represented by the value of x_0).

As monitoring networks become more extensive and emission inventories become more detailed in both space and time, superior relationships between emissions and concentration will be developed. This will enable the amount of emission limitation needed to attain and maintain a given air quality to be more accurately estimated. The means of attaining that emission limitation will continue to be primarily source category emissions limits which apply uniformly to such sources wherever they are located in the region. Whatever the relationship between emission and air quality, the problem will remain as to which sources to control and how much to control them in order to achieve the overall degree of emission limitation required by that relationship. Thus the technique presented herein should retain its value for some time to come.

Because the modified proportional model is primarily an emission accounting and projection scheme, its most appropriate application is for the exploration of alternative means of attaining and maintaining a given emission limitation. The effect of a particular source category emission limit may be quantified by estimating the percent reduction in total regional emission thus affected. This measure of effectiveness may be used when making cost-effectiveness comparisons between alternative control strategies.

If alternative control strategies do not involve substantial emission distribution differences, or if the pollutant in question is relatively insensitive to distribution factors (e.g., oxidants), then the relative impacts of the alternative strategies on air quality may be compared using the proportional model (see Figure 2).

[A note of caution concerning cost-effectiveness is appropriate here. Narrowly based cost-effectiveness calculations may produce appropriate inputs to air quality control strategy evaluation, but such inputs may not be the determining factors in choosing a control strategy. The indirect costs of implementing a particular emission control measure, the long range effects of air quality, and the measure's effectiveness in furthering goals aside from air quality improvement may weigh heavily in the evaluation of the measure.]

If no better method is available, then the proportional model may be used to estimate the amount of emission reduction needed in the region of interest. This procedure is sometimes carried to the point of estimating the emission reduction needed for a particular source category. This practice is questionable. In order to estimate one value of F_{ij}, all other values of F_{ij}, G_{ij}, and T_{ij} must be specified. Such specification can rarely be performed with high accuracy, so the estimated value of F_{ij} will be subject to considerable uncertainty.

Three further alterations of the modified rollback model may be mentioned: (1) The nonlinear relationship between hydrocarbon emission and oxidant concentration, (2) the treatment of man-made background concentration, and (3) the treatment of carbon monoxide.

Oxidants and Hydrocarbons

When the emitted pollutants are precursors of the offending pollutants for which control is desired, relationships which represent the atmosphere chemical reactions are required. Currently, these reactions are not yet sufficiently well specified to warrant use in the rollback model of other than a linear relationship as a best estimate of the degree of hydrocarbon emission limitation to attain the oxidant standards. If, as is likely, the relationship is non-linear and the nature of the relationships can be quantified, a term to account for the effect of limiting emissions of hydrocarbons on oxidant concentrations may be applied.

Man-Made Background Concentration

In the case where a portion of the background concentration is man-made, it is reasonable to assume that this concentration will decrease due to extra-regional emission reduction programs. The modified proportional model may be used as a first approximation of the expected decrease in the man-made background component.

If $B = B_n + B_m$

then $\frac{(B_m)_j}{(B_m)_o} \cong \frac{Q_j}{Q_o}$

Where B_n = Natural component of B

B_m = Man-made component of B

Q = Extra regional emission

The estimation of Q_j should follow the method presented earlier. The principal problem is the determination of the area for which Q_o and Q_j are estimated. This depends on the activity distribution in the section of the country in question, the direction or prevailing winds during periods of high background, etc. Common sense and "engineering judgment" must be used in making this estimate until more specific procedures are developed.

Carbon Monoxide

The concentration of CO varies markedly within an urbanized area. The predominant factor influencing this local variation is the intensity of motor vehicle activity on nearby streets. In order to better account for this local traffic effect, the modified proportional model may be altered thus:

$$x_T = x_L + x_R + B \tag{8}$$

$$\frac{x_L}{f\,(x_o - B)} = \frac{\sum_{i=1}^{n} P_i^* \, G_{ij}^* \, F_{ij} \, T_{ij}^*}{\sum_{i=1}^{n} P_i^*} \tag{9}$$

$$\frac{x_R}{(1 - f)(x_o - B)} = \frac{\sum_{i=1}^{n} P_i \, G_{ij} \, F_{ij} \, T_{ij}}{100\%} \tag{10}$$

Where x_O = Measured curbside CO concentration

x_T = Projected curbside CO concentration

x_L = Projected component of x_T due to local traffic emission

x_R = Projected component of x_T due to regional emission

$(1 - f)$ = Ratio of "rooftop" to "curbside" CO concentration

P_i^* = Percentage of CO emission contributed by mobile source category (i) to local traffic emission during the base year

G_{ij}^* = Growth factor through year (j) of mobile source category (i) in the immediate vicinity of the receptor in question

T_{ij}^* = Reduction factor in local traffic of source category (i) expected due to transportation controls through the year (j)

The other terms are the same as previously defined.

This model allows for the inclusion of local factors which may differ from regional factors. For example, local growth may be much less than regional growth; the proportion of light, medium, and heavy duty vehicles may vary from place to place within a region, and the effects of some transportation controls may vary with location.

The factor (1 - f) has been measured in several locations and has been found to vary between .1 and .4 depending on micro-geography. A value of .2 for (1 - f) and .8 for (f) is used as a best estimate when data on the ratio of "rooftop to curbside" concentration is unavailable.

Example of CO Model Use

The following data does not represent any particular place. It is selected from a composite of 26 regions in the United States in which high CO concentrations have been measured.

x_o = 31 ppm, second highest 8-hour average, 1970

B = 1 ppm

f = 0.8

P_{LDV} = 80% (LDV = light-duty vehicles)

P_{MDV} = 4% (MDV = medium-duty vehicles)

P_{HDV} = 6% (HDV = heavy-duty vehicles)

P_S = 10% (S = stationary sources)

F_{LDV} = 0.1 through 1980

F_{MDV} = 0.6 through 1980

F_{HDV} = 0.95 through 1980

F_S = 1.0

G_{LDV} = 1.3 (10 years at 3%/year)

G_{MDV}, G_{HDV} = 1.5 (10 years at 4%/year)

G_S = 1.6 (10 years at 5%/year)

$T=T^*$ = 1.0 (no transportation control)

P^*_{LDV} = 60%

P^*_{MDV} = 20%

P^*_{HDV} = 10%

$G^*_{LDV} = G^*_{MDV} = G^*_{HDV}$ = 1 (local traffic "saturated")

(NOTE: LDV = Light duty vehicles, $\leq$ 6000 lbs. gross vehicle weight

MDV = Medium duty vehicles, 6000 $\geq$ 14,000 lbs. gross vehicle weight

HDV = Heavy duty vehicles, $\leq$ 14,000 lbs. gross vehicle weight.)

If only regional emission changes are considered, then x_{1980} is estimated as

$$\frac{x_{1980} - 1}{31 - 1} = \frac{80 \times 1.3 \times 0.1 + 4 \times 1.5 \times 0.6 + 6 \times 1.5 \times 0.95 + 10 \times 1.6 \times 1.0}{100}$$

$$x_{1980} = 12.6 \text{ ppm}$$

If the full CO model is used, then x_{1980} is estimated as

$$\frac{x_L}{.8\ (31 - 1)} = \frac{60 \times 1 \times 0.1 + 20 \times 1 \times 0.6 + 10 \times 1 \times 0.95}{100}$$

$$\frac{x_R}{.2\ (31 - 1)} = \frac{80 \times 1.3 \times 0.1 + 4 \times 1.5 \times 0.6 + 6 \times 1.5 \times 0.95 + 10 \times 1.6 \times 1}{100}$$

$$x_{1980} = x_L + x_R + 1 = 7.3 + 2.5 + 1 = 10.8 \text{ ppm}$$

The estimation given by the CO model differs from that given by the regional proportional model due to the fact that:

1. The effects of peripheral growth are discounted in the CO model,
2. The effects of stationary source emission are discounted in the CO model, and
3. The effects of local vehicle mix are considered in the CO model.

The CO model will usually produce lower values than the regional proportional model for future CO concentration, unless the local CO emissions emanate from a disproportionately large percentage of trucks which are controlled less than passenger vehicles.

Summary

Several very basic assumptions, not always explicitly stated, are made when a rollback model is used:

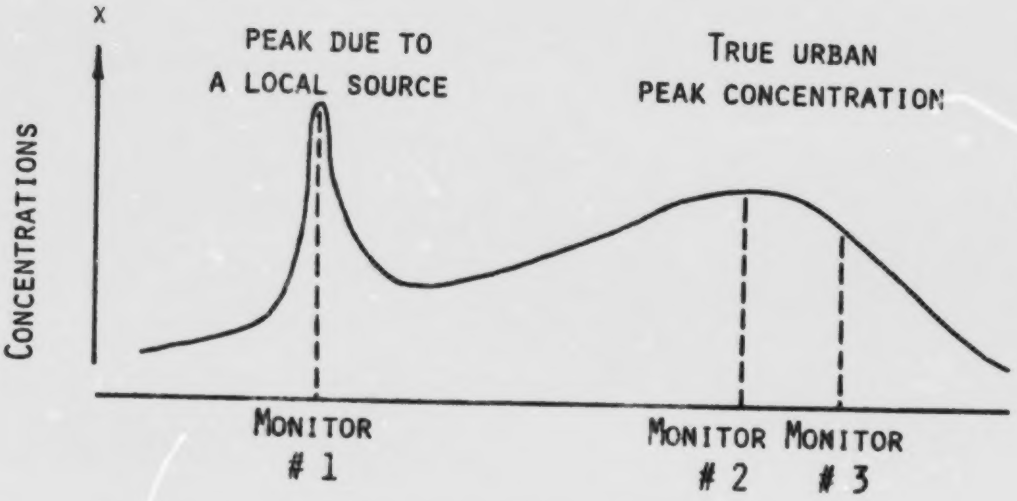
1. The indicator of air quality is representative of the air quality distribution over the region of interest.

2. The distribution of emissions in space and time is relatively stable over the projection period.

3. The meteorological and topographical characteristics of the area are stable over the projection period.

4. The average background concentration remains constant over the projection period.

The modified rollback model is fundamentally an emission accounting and projection scheme. It is convenient for exploring alternative means of attaining and maintaining a given emission limitation. If the emissions are homogeneously distributed, the relative impacts of alternative control strategies on air quality may be compared. It may be useful in making first approximations of the emission reduction required and in making crude estimates of the degree of control required or needed for specific source categories.


X
PEAK DUE TO A LOCAL SOURCE
TRUE URBAN PEAK CONCENTRATION
CONCENTRATIONS
MONITOR # 1
MONITOR # 2
MONITOR # 3

MONITOR # 1 IS INFLUENCED BY A LOCAL SOURCE
MONITOR # 2 MEASURES THE TRUE URBAN MAXIMUM
MONITOR # 3 MEASURES LESS THAN THE URBAN MAXIMUM

FIG. 1. EXAMPLE OF THE EFFECT OF MONITOR LOCATION ON MAXIMUM REPORTED CONCENTRATION.

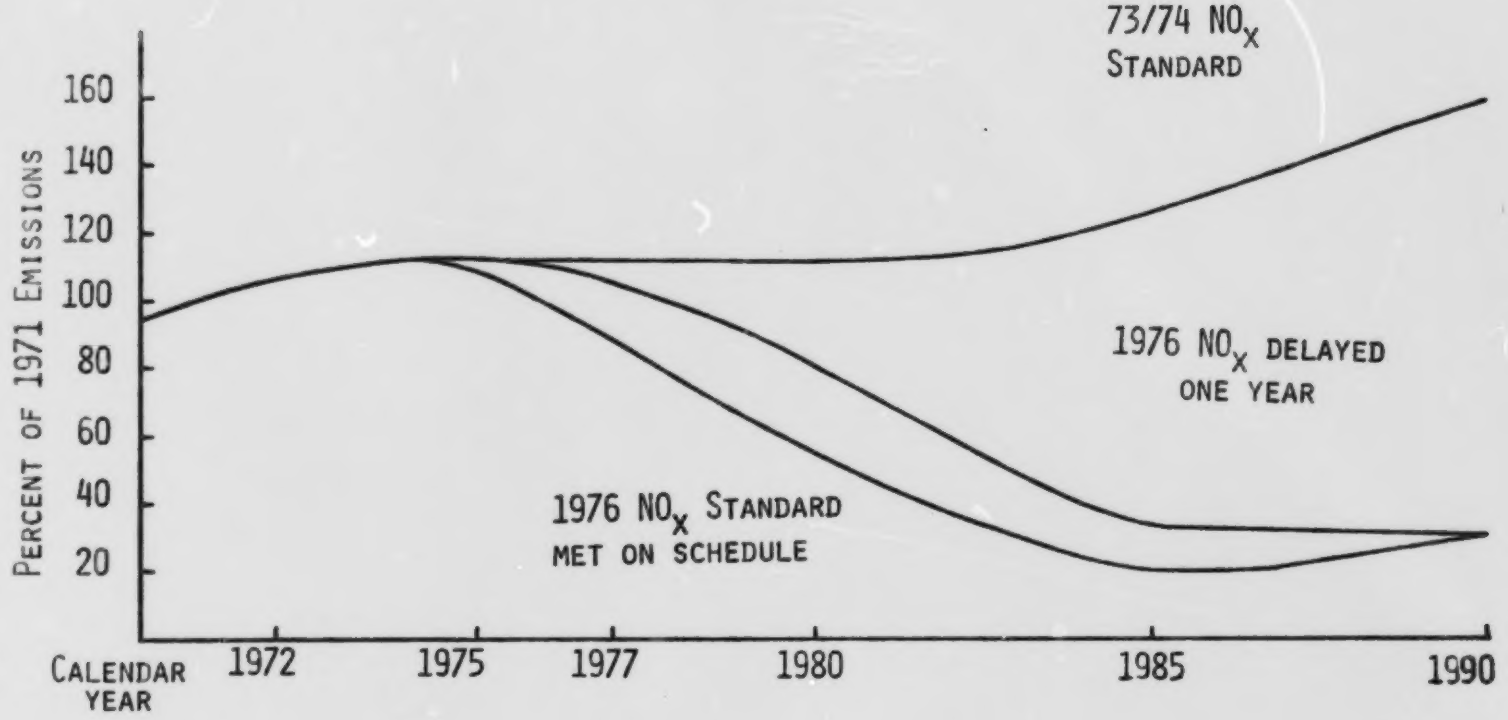


Fig. 2. Percent change in nationwide NO_x emissions from light-duty vehicles (LDV) as a function of time, emission standards and date of implementation of standards.

Acknowledgement

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Chapter 13

POINT - SOURCE PLUME MODELS

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

Point-Source Plume Models

by

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As indicated in the presentation on "Special Applications of Air Quality Models by EPA," point-source dispersion models are applied more frequently than any other form of dispersion models. Further, the point-source model is the basis for many multi-source urban models. Frequently, the multi-source models are essentially automatic data processing procedures which make repetitive calculations or iterations of the point-source model for many combinations of sources and receptors. So, in one form or another the point-source model is a frequently used analytical technique to estimate the impact of a source on the surrounding ambient air quality.

As Mr. Calder pointed out in his opening paper, a simple model of atmospheric transport and disperison of a pollutant from its source to a receptor shows that:

(1) Concentrations from a continuous steady source vary in direct proportion with the source strength or rate of emission.

(2) Concentrations vary approximately inversely as the mean wind speed.

(3) The average height and width of a pollutant cloud (a plume) vary little with wind speed. The height and width of a plume at a receptor is determined primarily by the distance from the source to the receptor and by the intensity of the atmospheric turbulence.

Atmospheric turbulence may be inferred from the vertical temperature gradient or atmospheric stability. A convenient classification of plume types relates the spreading of a plume to the stability or vertical temperature gradient. The behavior of plumes is indicated by the vertical temperature gradient, which in turn responds to the day-night diurnal cycle.

Air pollution meteorologists generally classify plumes into six types (Fig. 1):

(a) Unstable (looping).
(b) Neutral (coning).
(c) Stable (fanning).
(d) Stable below, neutral aloft (lofting).
(e) Unstable below, stable aloft (fumigation).
(f) Neutral below, stable aloft (trapping)

Knowing something of a plume behavior and the factors that determine the concentration of a pollutant at a receptor some distance from a source, a method is needed to quantify these factors so that a numerical model may be constructed.

It is apparent that the concentration at a receptor varies with the amount of pollutant emitted by the source. So the first step in constructing the continuous point-source model is to relate the concentration, which shall be called χ, to the emission rate or source strength, which shall be indicated as Q. The relationship can be stated as:

$$\chi \propto Q \tag{1}$$

The wind speed acts directly to reduce concentrations of the pollutant as it is emitted from the source by providing separation of the small puffs which make up the effluent plume. Doubling the wind speed doubles the spacing between the puffs and reduces the concentration by a factor of 2 if all other factors remain constant. (Figure 2)

The wind speed (U) may now be added to the relationship, which becomes

$$\chi \propto \frac{Q}{U} \qquad (2)$$

The horizontal and vertical spreading of the plume must yet be accounted for in a quantitative manner. As indicated, the width and height of the plume is a function of the turbulence or atmospheric stability. The turbulence causes the plume elements to fluctuate about a mean axis of the plume. This effect is shown schematically in Fig. 3.

If the character of the wind and the turbulence does not change, a short-term concentration will fluctuate but a mean concentration over a sampling period can be calculated. Figure 3 shows how the irregular fluctuations smooth out and predictable average concentrations are formed. The average concentration perpendicular to the plume axis, as represented on the right side of the figure, shows the peaked irregular concentrations in the instantaneous plume. The 10-minute average shows a smoothed, more regular boundary that may be assumed to enclose all the random plume puffs of the fluctuating plume. The 10-minute cross-plume distribution is wider and more regular but with a lesser maximum value than that of the instantaneous plume. The 2-hour case is even wider and flatter. These crosswind concentration distributions resemble the bell-shaped normal, or Gaussian distribution familiar to statisticians.[2]

A schematic representation of a plume's geometry is shown in Fig. 4.[3] The distribution of concentrations in the plume is schematically represented by the bell-shaped curves drawn for the horizontal and vertical planes.

The shape of a Gaussian distribution can be described quantitatively by the standard deviation.

Returning to the plume classifications, the shape of the crosswind concentration for the various plume types can be defined quantitatively by assigning a numerical value to a standard deviation.

Knowing that the plume type is related to the atmospneric stability, the plume width and height can be described quantitatively by relating the stability to a value for the standard deviation of the crosswind concentration. These relationships have been developed from a great deal of experimental data. It is sufficient to state that the numerical value of the standard deviaion is a function of the stability and the distance from the source to the receptor. The effect of plume spreading may now be added and the Gaussian dispersion equation expressed for the ground-level concentration at the plume centerline whose source is at the surface.

$$\chi = \frac{Q}{\pi \sigma_y \sigma_z \overline{U}} \qquad (3)$$

Where σ_y is the standard deviaion of the crosswind distribution of concentrations in the horizontal and σ_z is the standard deviaion of the vertical distribution.

Using meteorological and climatological data it is possible to assign appropriate numerical values to the wind speed, and the dispersion (σ) parameters. When the emission rate is also specified, it is possible to calculate a ground-level concentration. Additional adjustments can be made to account for situations where the pollutant is emitted from an elevated source and where the receptor is not directly downwind of the source.

The calculation will provide an estimate of a concentration averaged over a period of 15-60 minutes duration. It is possible to develop frequency distributions of wind speed, wind direction and stability from historical meteorological data. By making a series of calculations for each set of wind-stability conditions and weighting each calculation by the frequency of occurrence of each set of conditions and then summing the weighted concentrations, an estimate of a longer-term concentration can be made.

The basic point-source model with appropriate modifications for the specific problem has been applied by EPA for a variety of purposes. Some examples are:

The model has been used to evaluate new source performance standards for industrial sources. Many industrial facilities can control their emissions to within a fraction of a percent of the potential emissions. To do so becomes very costly, however. An attempt is made therefore to balance the need for control with the costs incurred. The impact of typical new sources is calculated (assuming the sources achieve control specified by the proposed emission standards) to determine the potential threat to ambient air quality. The model results at times have indicated that a slight relaxation of the standard may have a minimal impact on air quality, but the relaxation may effect substantial savings in control costs.

The model has been used to locate the areas where a source poses the greatest threat to air quality. The information is used to design air quality monitoring networks.

As the State Implementation Plans were approved it became obvious that several states were requiring controls on coal-fired power plants which were unlikely to be met by 1975. It appeared that an insufficient amount of low-sulfur coal would be available to meet the demand. Using the point-source model, analyses have been made of the impact of over 300 coal-fired power plants. It is expected that those plants which cause the greatest threat to ambient air quality standards or which are located in areas where other sources contribute seriously to contamination will be given high priority for the supplies of low-sulfur coal. Other plants may be able to make less drastic reductions in the sulfur content of the fuel or take other actions to reduce their emissions.

The National Environmental Policy Act requires that an environmental impact statement be prepared for all new facilities that are funded by public revenues. The point-source model has been used extensively to estimate the impact of a new facility on air quality. The results have become a part of the impact statements.

At numerous abatement and control hearings, estimates of the impact of a facility derived from the point-source model have been used in considerations of the need for control of specific point sources.

The question of the accuracy of the model outputs frequently arises. It is a difficult question to answer precisely. Each modeling effort is typically a case-by-case situation. The short-term concentration is particularly troublesome, because to obtain a precise result, it is important that input parameters are specified with precision. The meteorological parameters, the wind and stability are difficult to specify for periods of a few hours. The numerical values for the dispersion parameters, as was mentioned, are selected from curves fitted to empirical data. The source strength or emission rate of most facilities is not well established. As an example, in the United States, where the sulfur content of coal may average 3-5 percent, the day-to-day variation in the sulfur content may vary by a factor of 2.

Turner states that ground-level centerline concentrations should be correct within a factor of 3 for neutral to moderately unstable conditions out to a few kilometers and for unstable conditions in the lower 1000 meters with a marked inversion above out to 10 kilometers or more.[3] Dr. Klug is investigating the accuracy of these estimates using data collected in the Tennessee Valley. EPA is repeating his analyses using data collected in New England. It is believed a more definitive statement of the accuracy point-source model estimates will be possible during the coming year.

Slade in discussing the use of methods of making dispersion estimates placed the problem of the validity of estimates in proper context when he states in the preface of Meteorology and Atomic Energy 1968 "The reader should not expect to find hard and fast rules for the evaluation of a specific problem. The treatment of a practical situation usually involves the use of specific quantitative techniques along with a broad variety of assumptions engendered by the imperfect knowledge of the atmosphere and pollutant-producing device. Although these assumptions may be justified on scientific grounds, their selection can be rationally made only by someone with a broader range of experience and knowledge than can be gathered from even a careful reading of the following pages."[2]

In conclusion, to make the optimum use of these analytical techniques, it is prudent to engage a competent air pollution meteorologist. He understands the uncertainties inherent in the analytical procedures and he also has a keen appreciation of the many variations in weather conditions, their daily and seasonal frequency of occurrence and their effect upon the manner that pollutants are dispersed.

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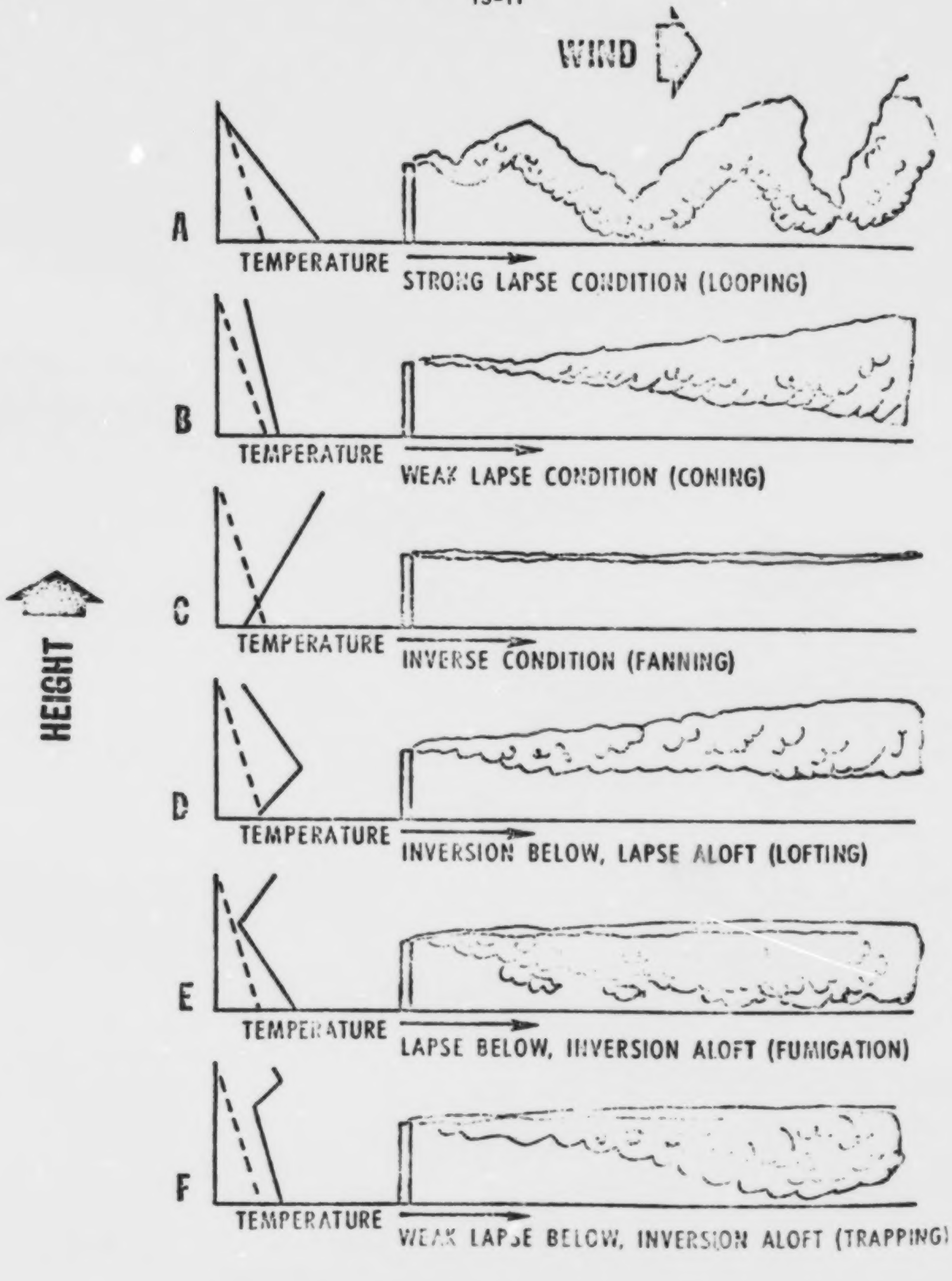
WIND
A
TEMPERATURE
STRONG LAPSE CONDITION (LOOPING)
B
TEMPERATURE
WEAK LAPSE CONDITION (CONING)
HEIGHT
C
TEMPERATURE
INVERSE CONDITION (FANNING)
D
TEMPERATURE
INVERSION BELOW, LAPSE ALOFT (LOFTING)
E
TEMPERATURE
LAPSE BELOW, INVERSION ALOFT (FUMIGATION)
F
TEMPERATURE
WEAK LAPSE BELOW, INVERSION ALOFT (TRAPPING)

Fig. 1. Types of Plume from Elevated Sources.

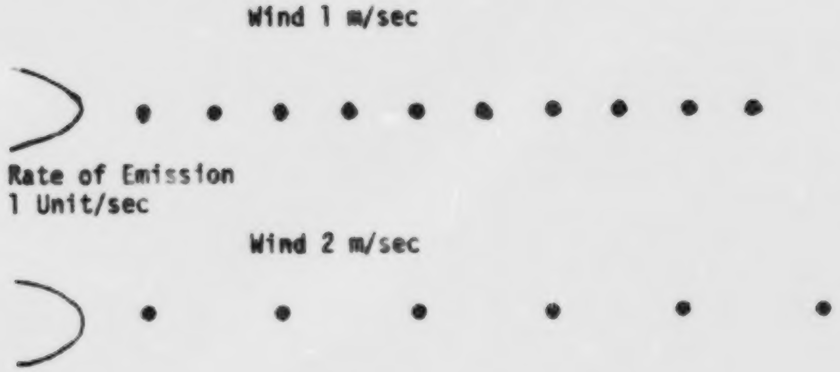
Wind 1 m/sec
Rate of Emission
1 Unit/sec
Wind 2 m/sec

Fig. 2. Direct Dilution by the Wind.[1]

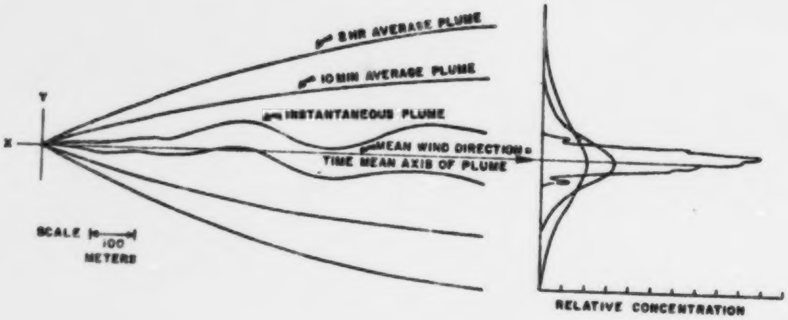
2 HR AVERAGE PLUME
10 MIN AVERAGE PLUME
INSTANTANEOUS PLUME
MEAN WIND DIRECTION
TIME MEAN AXIS OF PLUME
Y
X
SCALE
100
METERS
RELATIVE CONCENTRATION

Fig. 3. Instantaneous and Average Aspects of a Smoke Plume.[2]

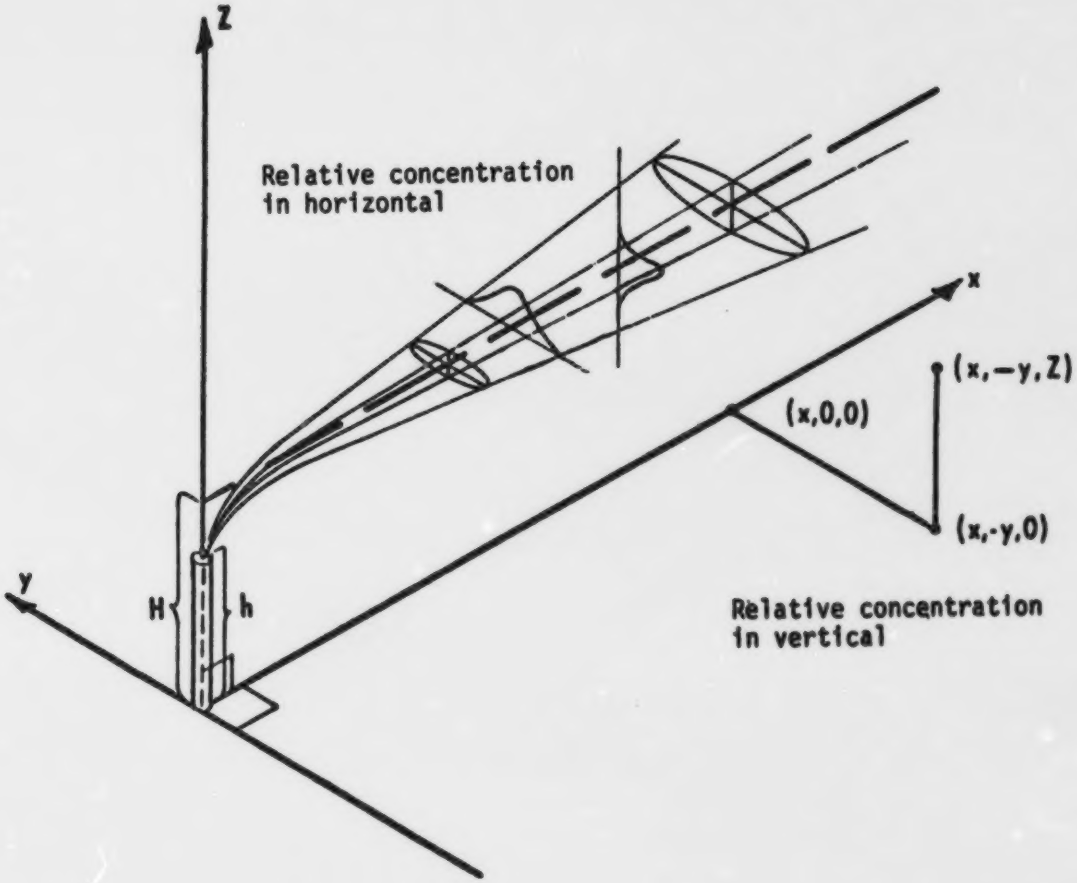
Z
Relative concentration in horizontal
x
(x,-y,Z)
(x,0,0)
(x,-y,0)
y
H
h
Relative concentration in vertical

Fig. 4. Geometry of a Plume from an Elevated Source.

Chapter 14

APPLICATION OF A MULTIPLE SOURCE URBAN MODEL

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

14-2

Application of a Multi-Source Urban Model

by

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Environmental Protection Agency

In the earlier discussion concerning the application of the Implementation Planning Program the use of a model was described for developing an implementation plan for the New York-New Jersey Metropolitan area. In that discussion, some early applications of models by the EPA were described. The applications were performed between 1966 and 1972. It was during these years that systematic attempts to quantify the individual air pollution problems for most urban areas in the United States began. Much earlier work had been performed, particularly in Nashville, St. Louis and Los Angeles. But these studies were to a major degree of a research nature. In the late 60's and early 70's, every state was required to develop strategies and tactics for protecting the quality of the air - and pass laws that would make the tactics and strategies legally enforceable.

The obvious way to obtain "clean" air is to enforce maximum control of all sources of pollutants. However, for economic and technical reasons, maximum control is seldom feasible - nor often truly necessary - except in cases of certain hazardous pollutants, such as beryllium, mercury, asbestos and perhaps a few others. Thus it is appropriate to use engineering judgments to select the optimum techniques to attain a desirable level of air quality.

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Engineering judgments are limited to the understanding of control of individual sources. Such judgments do not encompass the impact of simultaneous emissions from many individual sources. A tool which relates pollutant emission rates to air quality is required. Such relationships can be used to identify the sources which, if controlled, can enable air quality to be enhanced with least economic and social disruption and with least impact on the legal system. The latter includes the entire enforcement effort.

The tool used is an air quality or dispersion model to simulate the action of atmosphere in dispersing, modifying, and transporting pollution from its source to any other point, usually called a "receptor." There are at least 15 models that are now available in the United States to assess general urban air pollution problems. They vary greatly in their complexity, in their data requirements, in their attempts to account for such problems as atmospheric chemical reactions, topography, land-sea effects, change in wind and stability with height and with time, etc. The model that is chosen depends on the nature of the pollutants, the adequacy of the input data, the computational resources (how big is the computer, if a computer is available), and the adequacy of the air quality data to determine how well the model simulates the problem at hand.

Turning back to the 1966-1972 time period, the EPA and its predecessors had two classes of problems. The first concerned a situation where pollution emitted in one state was alleged to degrade air quality and affect the health and welfare of citizens of another state. The second concerned the evaluation of state implementaion plans for attaining air quality standards.

Evaluation and often the development of appropriate control tactics were required within a few months. At the same time, the states were undertaking programs to procure an emission and air quality data base. In summary, a detailed data base demanded by a sophisticated model did not exist. There was no real hope of assessing 24-hour concentrations realistically; a long-term average concentration model was the most appropriate analytical tool available.

The long-term dispersion model that was applied was appropriate for the so-called stable pollutants: suspended particulate matter and sulfur dioxide. Since it was a long-term model, it was concerned with average air quality. It provided an estimate of the impact of all sources on each of a set of receptors. It provided no information of the impact during a specific set of circumstances.

The model selected allowed the input data to be aggregated or summarized. Though a great amount of data was required, the detail required was minimized. The emission data were input in terms of average annual emissions; the meteorological data were summarized into frequency of occurrence of classes of wind direction, wind speed and stability (there were 480 such classes); the air quality data, to evaluate the performance of the model, were annual averages.

A grid was overlaid on the area of concern. Each individual source which emitted 100 tons of the pollutant annually was called a "point" source and located precisely. All emissions other than from point sources were called "area" sources and apportioned among the source grids. Receptors were located, as many as possible at sites where air quality was measured. The contribution of each point and area source to the degradation of air quality at each receptor was then calculated for each of the 480 meteorological classifications. The individual contributions at each receptor were weighted and summed to provide a long-term average air quality. The lack of detail was undesirable. Nevertheless, the discrepancies between air quality calculated using the model and the observed air quality were not solely caused by the inadequacies of the model. It is known that errors in the input data discussed below, also contributed significantly to the errors.

Every attempt was made to insure that the data (emissions, meteorological, air quality) which were used in the model were complete, concurrent and correct. Any model is sensitive to the accuracy of input data. For this reason, inherent data problems must be understood and the data itself critically scrutinized before a model can be applied to any area.

Emission Data:

The source data used included pollutant emission rate, stack parameters, the size of area sources and source location. Emission rates were annual or seasonal averages, did not reflect diurnal variations, and were developed from engineering emission factors. Point sources generally included sources with emissions greater than 100 tons per year. The stack parameters were routinely obtained through the source inventory process. Missing point source data were estimated from engineering information on stack parameters, characteristics, type and size of the facility. Area sources included all sources, e.g., residential and commercial space heating, open burning, mobile, etc., which were not individually large enough to be considered point sources. The geographical size of the area sources, usually one to ten kilometers on a side, was adjusted so that the detailed spatial variation in emissions could be delineated. Small area-sources were used where emissions were dense and spatially, highly variable. The Universal Transverse Mecator Grid System was used to locate all sources to the nearest 100 meters.

The model was particularly sensitive to errors in emission rates and to errors in the location of sources. Errors in the stack data, which affect plume rise computations, had a significant effect if the source was close to the receptor. Aerodynamic downwash was not considered.

The model estimates indicated concentrations due only to air pollutant emissions from sources located within the area modeled. If the air quality data indicated the existence of "background" concentrations, natural or otherwise, such concentrations were added to the estimates.

Meteorological Data:

Meteorological data representative of the area were used to determine the joint frequency distribution of meteorological conditions; data of the type collected at a National Weather Service Airport Station were preferred. The model considered five stability classifications, sixteen wind directions and six wind speed classes; a total of 480 possible weather conditons. The five stability classes include a range from very unstable afternoon conditions to stable nighttime conditions. Stability was determined by the estimated amount of net solar and/or terrestrial radiation and wind speed. Wind direction was specified by the standard compass directions. Wind speed was indicated by six standard speed classes, e.g., 0-3, 4-7, 8-12, 13-18, 19-24, and greater than 24 mph; the speed representative of each class was determined by the class mid-point. Average afternoon mixing height, which defines the atmospheric layer in which vertical mixing occurs, was applied. Mixing height data were derived from National Weather Service (NWS) radiosonde observations taken at the NWS station representative of the area being modeled.

The selection of a meteorological sampling site which can provide the data necessary to describe transport and dispersion in the area being modeled was difficult. Generally, the best source of data was an NWS airport station, where the necessary meteorological parameters were routinely observed and disseminated. Airport data are collected in rural or suburban surroundings and may not be truly representative of an urban area; nevertheless, they were frequently the best available. In cases where there was a significant difference in the horizontal or vertical transport and dispersion over an area, additional meteorological data was applied to recognize in a gross manner the topographical influences.

Air Quality Data:

It was desired to determine the general reliability of the results and to identify the areas and circumstances that the model estimates were least reliable. To do so the model estimates were compared with observed air quality data.

Hopefully air quality data used to verify the model was collected during the time period that emissions and meteorological data were collected. In addition, data were needed from a sufficient number of locations to identify the highest and lowest concentrations and to define gradients of air quality. Even long-term air quality data were precise to only 10-15 percent. Different sampling techniques were used by the several air pollution control agencies. Some samplers were located in areas where buildings created anomalous flow which affected the sampled data. Some were located on roofs of 4-story buildings. In no case was the data collected for these studies tailored to the development of a dispersion model or development of strategies. The air quality data were obtained from attempts to identify the flow of pollutants from one area to another or to substantiate general levels of pollutant concentrations. Little consideration had been given in most cases to the selection of optimum sampling locations. Convenience in servicing the equipment frequently dictated the location. To assure that the comparisons between observed and predicted air quality were valid, the data were carefully reviewed to insure that any factors which might have created spurious data were known.

Application of Model

The model was applied to 18 urban areas for two pollutants, SO_2 and particulate matter. Periods of two months to a year were considered. The source data was often composed of 100 or more point sources and several hundred area sources. The area sources were as small as 1 kilometer on a side, depending on the detail of the inventory available. The larger area sources were 20-50 kilometers on a side. The larger area sources were used to handle emissions from suburban or rural areas which did not cause high concentrations in the urban center, but contributed to the background of pollution entering the area.

Frequently, the source data were obtained from routine emission inventories developed to determine the types, quantities and locations of pollutant emissions in the area. The emission rates were generally based on emission factors and material processed or fuel consumed. Little of the data were based on actual emission samples taken in the stack. The point source data consisted of an address, an emission rate, and possibly a stack height only. Since it was necessary to specify all source receptor locations in terms of the U.T.M coordinate system, all the sources were located on an appropriate map and the coordinates specified.

Physical stack data were seldom available in detail. Power plants were the only type of soruce that could be relied on for detailed data. In some cases where no data were available it was necessary to estimate a plume rise from previous experience based on source-type or size.

Area source emissions generally were based on fuel use and traffic data for a Standard Metropolitan Statistical Area (SMSA) and appropriate emission factors. Emissions for various zones within the SMSA were computed. Then, subjectively, the zones were overlayed with a grid network of squares and emissions were estimated for each square area. (NOTE: The EPA has established a National Air Data Bank. It is now possible to obtain the location, characteristics, and emission rate of point sources and the total emissions from the non-point sources of each of the Nation's 3000-odd counties. Similarly all air quality data collected by air pollution control agencies are archived. The location of each sampling point is precisely identified.)

The seasonal and annual average air quality data varied considerably in type, quantity and quality. Generally, 15-30 sampling sites were available in each urban area; the fewest number was 5. The exclusive source of particulate matter data were Hi-vol samplers, operated for 24-hour periods. Data were available from a variety of SO_2 sensors, including several models of continuous samplers, bubblers and sulfation candles. Sulfation data were related to SO_2 measurements by comparing sulfation and SO_2 samples at a limited number of locations and developing a conversion factor. Generally, the relationship was approximately 1 mg SO_3/cm^2-day = 100 $\mu g/m^3$ of SO_2.

The meteorological data were most often typical airport station data. The direction and speed frequencies were readily available and the stability was determined from a technique suggested by Turner. In cases where only wind data were avilable and stability could not be estimated, it was assumed that Pasquill Type E stability occurred during the nighttime hours and Pasquill Type C stability occurred during the daytime. In one case stability classes were empirically determined from temperature differences and associated wind speeds on a tower.

In most applications, it was assumed that the terrain was flat and level. One meteorological instrument near the surface was assumed adequate to describe wind flow and stability in the lowest layers of the atmosphere. When this was obviously not the case, as in complex terrain, simple modifications were made in the model to account for a change of meteorological regimes. In valley terrain when sources were located so that some emitted pollutants below and others at or above ridge level, one set of wind data was used to describe transport and dispersion from the valley sources and another from the ridge-level sources. Under very light wind conditions at night, it was assumed that emissions at below ridge level were not transported from the valley. When receptors were available at both valley and ridge levels, adjustments were made to the sources' effective stack heights, to account for the difference in elevation.

As indicated, the air quality data must be reliable, or erroneous conclusions about the accuracy of the model may be made. At times some of the air quality data available was so suspect that it was discarded. In every area there was at least one sampling site at which the observed air quality data was either questionable or the estimated concentration was eminently more reasonable. The data may have been degraded by a shortened sampling period or excessive missing data. In some cases the exposure of sampler was very poor. In others the value reported was so extreme that it could not be rationalized nor reproduced with the emissions available for the model. Air quality data were never discarded, however, without as thorough an investigation as time and manpower would allow.

In some cases the model was not validated at certain sites because it was known that the emission inventory was inadequate. This was especially true of outlying areas and sites near very large sources whose emissions were not well established. On occasion it was necessary to discard sampling sites from consideration because it was known that the meteorological data were not representative of transport and disperion in the vicinity of the site.

Model Verification

Unfortunately the amount of air quality data was usually limited. Therefore, detailed, statistical tests of model accuracy were not possible.

The two best tests became a regression analysis and a comparison of the spatial distributions for the measured and estimated concentrations.

Correlation and regression analyses provided an indication of the overall accuracy of the model in a comparison of the estimated vs. measured concentrations and indicated the magnitude of errors at individual locations. Comparison of the spatial distributions indicated the capability of the model to represent the variation of air quality over an area. The two techniques when considered together provided indication of the accuracy of the model estimates. Because of the large number of areas which were modeled, only the regression analyses are presented.

The overall results of the application of the model to 18 areas are presented in Table 1. The range of correlations between observed and estimated concentration is shown to be 0.50 to 0.94. All correlations were significant in that they exceed the correlation coefficient that could be expected by chance at a 95 percent confidence level. For particulate matter a correlation coefficient greater than 0.7 was generally obtained. In areas not affected by terrain, a correlation greater than 0.8 resulted. For SO_2 a correlation of at least 0.8 was obtained in most areas. For individual points, the model predictions were within a factor of 2 of the measured air quality.

A summary of the modeling effort, the magnitude of each problem area and the results are shown in Table 1.

Summary

The application of a rudimentary Gaussian multi-source model provided helpful data on the distribution of "stable" pollutants in several urban areas. It provided gross indications of the geographical extent of the more serious contamination, identified many of the major sources of contamination and gave a gross indication of the degree of emission control needed. Surprisingly, on several occasions results indicated serious deficiencies in the emission inventories.

Current Activities

Currently, the EPA is using more sophisticated models which can take advantage of the more detailed emission inventories becoming available. Modest efforts have been made to account for topographic factors and for the wind fields and turbulence intensities typical of an urban area (in contrast to suburban-rural environments where most official meteorological data are observed). A great need exists for models which can routinely handle the reactive pollutants. These pollutants emanate largely from the automobile and other mobile sources. A model exists for CO emissions from automobiles, but the problem of obtaining realistic emission inventories of mobile source emissions makes this model difficult to use on a routine basis. Simple models have recently been devised for use in air quality maintenance and assessing the impact of so-called indirect sources, e.g., sports complexes, shopping centers, amusement parks, parking facilities and the like.

Table 1. Summary of Operational Urban Air Quality Modeling

City	Year	No. of Sources Point	No. of Sources Area	No. of Valid Samples TSP	No. of Valid Samples SO_2	Correlation Coefficient TSP	Correlation Coefficient SO_2
Boston	1970	384	459	9	11	0.89	0.78
Buffalo	1969	341	304	25	30	0.81	0.73
Chattanooga	1967-68	---	---	--	--	----	----
Chicago	1968	459	169	54	38	0.72	0.50
Cincinnati	1969-70	127	380	41	7	0.69	0.92
Denver	1968	40	93	19	12	0.60	0.78
Detroit	1967-68	450*	2000*	26	37	0.89	0.81
Ironton-Ashland-Huntington	1965-66	40	90	6	10	0.92	0.78
Kansas City	1966-67	129	200	8	21	0.85	0.88
Kansas City	1969	181	207	27	--	0.71	----
Louisville	1970	168	108	16	4	0.79	0.95
Milwaukee	1970+	203	215	25	9	0.80	0.71
New York	1969	678	863	113	75	0.62	0.89
Philadelphia	1968-69	945	276	12	50	0.92	0.90
Port Huron	1967-68	450*	2000*	21	23	0.82	0.84
St. Louis	1968	115	312	15	23	0.74	0.75
Seattle	1969	180#	250#	5	--	0.99	----
Steubenville	1968+	90	260	15	22	0.77	0.60
Tacoma	1969	180#	250#	5	5	0.93	0.95
Washington, D. C.	1969	180	686	23	5	0.83	0.94

*Total of Detroit and Port Huron Sources.

#Total of Seattle and Tacoma Sources.

+Less than 12 Months.

Chapter 15

THE USERS' NEED FOR PRECISE DESCRIPTION AND VERIFICATION OF A MODEL

by

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5th Meeting NATO/CCMS Expert Panel
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Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

THE USERS NEED FOR A PRECISE DESCRIPTION AND VERIFICATION OF A MODEL.

As a uder I represent the Greater Copenhagen Air Pollution Committee which runs some twenty measuring sites in the Copenhagen area. On each site is placed an 8-port OECD-apparatus measuring daily values of sulphur dioxide and soot.

A user in this connection is a person who is not concerned with constructing air pollution models either because he has no interest in such work or because he is lacking the time. It is his interest to use an air pollution model in the control and management of the air quality in a certain area. The model itself is to him more or less a black box and his needs are not a detailed description of what is inside the black box but a clear and precise description of the conditions for using the model and the outcome.

Important in the black box description of the model is precise details on output and input. Here it should not be forgotten to tell the plain facts about the model in a simple manner such as the answers to questions like these which all refer to the output: Is the output an area average concentration or a single location concentration? Can single location concentrations be given for the grid points only or for any location? Can the model predict concentrations for different heights above ground? Can the model give outputs hour for hour or only for longer time-intervals?

Concerning the input data there should of course be an exact statement of what is needed.

The models ability to predict air pollution concentrations is the main justification for using the model and good information on how well a model can do this job is very important for the user. Telling about a models ability to depicture reality presupposes that we have a measure for the agreement between calculated and observed data. I feel that there is a need for a better measures than I have seen in use hitherto. The often used correlation coefficient is in my opinion not a suitable measure.

In statistics the correlation coefficient is basically the fifth parameter needed for the specification of the twodimensional normal distribution. If we are dealing with data from a twodimensional normal distribution the use of the correlation coefficient is all right. If we are not the use is not justified because the interpretation of the correlation coefficient is very uncertain. This is not serious if an actual calculation comes out with a correlation coefficient of 0.99 but if the result is 0.6 it is.

It may well be disputed to what extend the output from the model are stochastic variables. This is interesting because the function of correlation coefficient is to describe the relationship between two stochastic variables. The models I know produce one and only one set of outputdata for a given set of inputdata. They are deterministic and there are no stochastic elements in the model itself. The output can then only be considered as stochastic variables if the inputdata can. Source strength data are hardly samples from stochastic variables. Meteorological data taken over long periods may be considered as stochastic data but is this justified for data from a short period like a day, a week or a month? You will understand I do not favour the use of the correlation coefficient and I strongly recommend the use of a better and particularly more informative measure for the agreement between the model and the reality.

A far better measure in my opinion is to calculate the root mean square difference between observed and calculated values. This measure can be used directly for the calculation of confidence limits for the model and it is far less sensitive to range of the test data than is the correlation coefficient. Anyway modelers should work out proper measures for the agreement between model and reality and present the reasons for their choice. Efforts are not wellbalanced when you use many hours of modelmaking and getting emission data and then use poor measures of fit.

It is of course not sufficient to inform about the agreement between the model and reality expressed with the aid of a suitable measure for goodness of fit. It is also necessary to present the background of the test so it might be possible to judge the cause if the agreement is not as good as desirable. Insufficient agreement may be due to:

1. The source strength data
2. The meteorological data
3. The observed data
4. The model itself

In the first hand the user is not interested in details of the model because he first vants to see if the lack of agreement is due to other factors than the model itself. Is this the case there is little point in improving the model.

About the source strength data I would like to know how the emissions are distributed among point and area sources and I would like a short description of the major point sources. It should be told how the source strength variation during the year and the day is estimated and introduced into the model. There should also be a clear statement of the approximate accuracy of the survey data.

In presenting the meteorological conditions it is of course valuable to know that period of time they cover but it is more interesting to know if the period was typical or not typical and whether the period covered a narrow or a broad range of meteorological conditions and the incidence of stagnant conditons and similar information.

The range of the observed data should be given since a model tested over a broad range of real data is more trustworthy than a model tested only over a small range. The observed data will contain random elements (at least measurement errors) that model of today never will be able to account for. So even with most detailed information on sources and meteorological conditions we can not make perfect predictions. That means that the variance of the observed concentrations around the calculated concentrations should for a given model not be compared with a variance of zero but rather with some minimum variance representing the above mentioned random elements.

Observed and calculated values may not correspond exactly to each other. Maybe the model calculates an area average which leaves you with the problem of how well single location measurements represent the area average. Maybe the model calculates grid point concentrations and your measuring location is not a grid point and you have the same problem again. It is difficult to judge the magnitude of deviation because data that tells about the variation of contrations in space within distances of 1 kilometre of less are scarce. This is in contrast with the abundance of data on the variation og concentrations with time. I strongly feel it should be valuable to have a better knowledge of the spatial variation of urban air pollution concentrations within short distances.

It has been claimed that simple models often do just as good or slightly better predictions than do more complicated models. Users in the administration of air quality are not interested in using more complicated models than necessary. They need good information about different types of models in order to choose the one suitable for their purpose and I have tried to outline some the information I think is usefull.

So, Dear modelers, please provide users and administrators with good and precise information about your models.

Chapter 16

LINE SOURCE MODELING

by

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5th Meeting NATO/CCMS Expert Panel
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Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

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LINE SOURCE MODELING

by

D. BRUCE TURNER

ABSTRACT

This paper discusses estimation of air pollutant concentrations from line sources such as highways and airport runways. Emphasized is the Gaussian plume approach applicable when there is undisturbed horizontal flow from the source to the receptor. Results are given for an example of the estimation of particulate sulfate concentrations from motor vehicles. Sensitivity to atmospheric stability and to the angle between wind direction and source orientation is shown. Sufficient comparisons have been made with field measurements to give some degree of confidence in the use of this model.

INTRODUCTION

This paper discusses the estimation of air pollution concentrations that result from line source emissions. Highways and airport runways are examples of such line sources. To estimate concentrations from these line sources, several different approaches have been used. These include use of Gaussian models and of cell models. Inputs to the models require information concerning the source geometry and its emissions, the meteorological conditions, and also the location of the receptor points. One of the primary needs for a line source model is to estimate concentrations from linear highway segments. These estimates are used in preparing environmental impact statements. Of major interest for impact statements are the meteorological conditions and angle of the wind with the roadway that lead to the highest concentrations.

An additional use of line source models is to determine the environmental impact of aircraft emissions from runways and taxiways.

APPROACHES

There are several different approaches to simulating dispersion from line sources. The approach that will be emphasized here is the use of Gaussian dispersion models. The Gaussian models assume that the distributions of pollutants in the crosswind and vertical directions are Gaussian or bell-shaped distributions. The Gaussian approach is limited to situations where the wind flow is horizontal and parallel to the ground, and a single representative wind speed can be chosen.

Situations that have been considered using the Gaussian model are "at-grade level" roads and also roads in "cut-sections." In the case of the "cut-section" roadway, it is assumed that the flow above the cut is essentially horizontal and estimates are only made for receptor points outside the cut.

Depending upon the angle between the wind direction and the roadway, and also upon the length of the roadway, either simple formulae or numerical integration procedures are used to estimate the concentrations at receptors. These are discussed below.

In applying the Gaussian model to highway segments, a separate line source and emission rate are used for each lane of traffic. To account for the initial dispersion in the turbulent wake behind each vehicle, an initial distribution of pollution is also assumed.

Air quality estimates are needed for averaging times of 1 hour or longer because of the averaging times of the air quality standards. Therefore, emissions averaged over hourly time periods are used. The averaging is done by determining total vehicle flow for each hour and the appropriate emission factor to obtain the average emission over each one-hour time period. Different emission rates can be used for each lane of traffic based on the number of vehicles using that particular lane.

Other approaches, such as the grid approach, as used in the EXPLOR Model, (Sklarew, Fabrick, and Prager, 1972) have also been applied to line sources. Cell models, using diffusivities for the dispersion, can account for variations in flow and the increase of wind speed with height. However, these will not be discussed in this paper.

INPUTS TO THE MODEL

There are three important inputs to the line source model. First, the location of the source and the emission rates must be known. In the case of a highway segment the coordinates of the end points of the segment, the number of lanes, the total width of the highway, and the width of any median are required. Emissions for each lane separately are entered as grams per second per meter of length. This line source emission rate, q_ℓ, can be found if the emission factor EF (g veh^{-1} km^{-1}) and the traffic volume TV (veh hr^{-1}) are known. The following equation similar to that from Zimmerman and Thompson (1974) is used:

$$q_\ell \ (\text{g sec}^{-1}\text{m}^{-1}) = \frac{\text{EF} \ (\text{g} \ \ \text{veh}^{-1} \ \text{km}^{-1}) \ \text{TV} \ (\text{veh hr}^{-1})}{1000.(\text{m km}^{-1}) \ 3600 \ (\text{sec hr}^{-1})}$$

$$= 2.78\text{x}10^{-7} \ (\text{EF}) \ (\text{TV})$$

A value for the emission factor can be obtained from the Second Edition of Compilation of Air Pollutant Emission Factors (EPA, 1973). When vehicle speed is known and different from that used in the reference, a multiplier correction factor is used.

The second category of input is meteorological conditions. Wind direction, wind speed, stability class, and mixing height are required for each hour. Since mixing height is the top of the neutral or unstable layer, it is not a valid concept for situations where stable conditions exist in the layer of atmosphere near the ground. Therefore, a value for mixing height is not considered for stable conditions.

The third classification of input is the location of receptors. The East and North coordinates and the height above ground (usually zero) are needed.

Calculation of Concentrations

For the special situation of the wind direction perpendicular to the line source with the end points of the line at some distances from the location of interest, the Gaussian Model is a simple equation:

$$\chi = \sqrt{\frac{2}{\pi}} \frac{q_\ell}{u \, \sigma_z (x + a)} \qquad (1)$$

This and all other equations presented here are for the case where both the line source and the receptor are at ground-level. χ is the concentration,

q_ℓ is the emission rate, u is the wind speed, and σ_z is the dispersion parameter value dependent upon distance from the source and stability class. The distance from source to receptor is x. a is the virtual distance to give the required initial σ_z (discussed below).

Calder (1973) has given a modified equation to use when the line source can still be regarded as infinite in length but the wind deviates from the perpendicular. Deviations as much as 75° from the perpendicular can be handled in this way for very long line sources (about 15 to 20 km). The equation used is:

$$\chi = \sqrt{\frac{2}{\pi}}\ \frac{q_\ell}{\sin\alpha\ u\ \sigma_z(x + a)} \qquad (2)$$

where α is the angle between the wind direction and the orientation of the line source and x, which is the distance from the receptor to the point on the line source directly upwind, is found from:

$$x = d/\sin\alpha$$

where d is the perpendicular distance of the receptor from the line source. If more than one lane of a roadway is being simulated, the equation must be applied to each lane independently and the resulting concentrations summed.

When the wind direction is close to that of the line source, or the line source can no longer be regarded as infinite so that end effects may occur; Calder's approximation is no longer valid. The calculation of concentration must be made by a simple numerical integration of the Gaussian plume point source equation over a finite length. The coordinates of the end points of a line source of length L extending from point A to B (see figure 1) are R_A, S_A and R_B, S_B. The direction of the line source from A to B is β. The coordinates R, S of any point along the line at the arbitrary distance ℓ from point A is given by:

$$R = R_A + \ell \sin \beta$$

$$S = S_A + \ell \cos \beta$$

Given a receptor at R_k, S_k, the downwind distance, x, and the crosswind distance, y, of the receptor from the point R, S for any wind direction θ is given by:

$$x = (S - S_k) \cos \theta + (R - R_k) \sin \theta$$

$$y = (S - S_k) \sin \theta - (R - R_k) \cos \theta$$

Since R and S are functions of ℓ, x and y are also functions of ℓ.

The concentration, χ from the line source is then given by:

$$\chi = \frac{q}{u} \int_0^L \frac{\exp(-y^2/2\sigma_y)d\ell}{\pi\sigma_y(x+b)\sigma_z(x+a)}$$

where a and b are the virtual distances required to produce the initial σ_z and σ_y respectively.

The trapezoidal approximation to the integral is found by the following. Let $\Delta\ell = L/N$

$$\chi = \frac{q\Delta\ell}{u} \left[\frac{1}{2}(f_o+f_N)+ \sum_{i=1}^{N-1} f_i \right] \tag{3}$$

where:

$$f_i = \frac{\exp\left\{\dfrac{-y^2[i\Delta\ell]}{2\sigma_y^2(x[i\Delta\ell]+b)}\right\}}{\pi\,\sigma_y(x[i\Delta\ell]+b)\,\sigma_z(x[i\Delta\ell]+a)}$$

For a given initial choice of the interval length, $\Delta\ell$, the calculation is then interatively repeated with twice the number of intervals, that is, with $\Delta\ell/2$, $\Delta\ell/4$ ..., until the concentration estimates converge to within some specified limit of accuracy. This value then represents the true value of the integral.

Figure 2 gives guidance on which equation or procedure to use for receptors near a specific line source. For winds perpendicular to the source, equation (1) can be used over a wide area. Equation (2) can be used over a smaller area. The size of both of these areas increases with length of the line source. Also the angular range for which equation (2) applies, changes somewhat with source length.

The initial dispersion caused by the downwash or wake effect behind each individual vehicle is considered in the model by assuming an initial σ_y (horizontal dispersion parameter) value of 3 meters, and an initial σ_z (vertical dispersion parameter) value of 1.5 meters at each point along the line source. This is depicted in Figure 3.

SPECIFIC EXAMPLE

The example discussed here relates to particulate sulfate concentrations produced by automobiles. Most gasoline marketed in the United States contains a small amount of sulfur. In order to meet automobile emission standards for carbon monoxide and hydrocarbons, catalytic converters are scheduled for use on a number of 1975 model-year automobiles. The converter will oxidize carbon monoxide and hydrocarbons to water vapor and carbon dioxide. It will also oxidize the sulfur in the exhaust to sulfur trioxide which will rapidly convert to sulfuric acid due to the high humidity in the exhaust. Sulfuric acid mist and other sulfate aerosols will result.

Measurements of atmospheric sulfate have been related to adverse health effects in various studies (Finklea, 1973). It is therefore desirable to estimate sulfate particulate levels at receptor locations near busy roadways. Since associated health effects have been compared with 24-hour measured air quality levels, it is desirable to make the estimates with the model for up to 24 hours.

An estimate of emission rate of sulfate from catalytic equipped vehicles was first obtained from the mobile source air pollution control experts. Computations were then made on the assumption that 25% of the vehicle miles traveled on the roadway segment were by vehicles equipped with catalytic converters. A segment of expressway, 10 lanes in width, (43 meters wide including a 3 meter median) and 2 kilometers in length was chosen as the source. Traffic flow rate at the busiest time of day was assumed to be 2,000 vehicles per hour per lane.

Estimates of hourly concentrations were made for a day having rather typical meteorological conditions, and for a day with adverse meteorological conditions. Receptor locations, perpendicular to the mid point of the 2 km highway, were considered at 3, 50, and 500 meters away from the downwind edge of the highway. Computations were made with the wind perpendicular to the highway segment. Computations were then made varying the angle of wind direction to the highway in order to determine what angle produced the maximum concentration at each specific receptor. The results of these short term estimates with an everaging time of one hour are shown in Table 1.

Computations of 24-hour sulfate concentrations at each receptor were then made, varying both meteorological conditions and the volume of vehicles, hour by hour. Realistic vehicle flow rate variations were obtained from highway experts. The hourly meteorological conditions used were from a 24-hour period of airport data. This 24-hour period was selected for its light wind speeds, stable conditions, and small variability in wind direction. An orientation of the highway segment was chosen so that there was some cross-expressway component of the wind in the same direction during most of the 24 hours. The temporal variations in concentrations at the various receptors are shown in Figure 4. Average estimated 24-hour concentrations during this period at the receptor distances of 3, 50, and 500 meters are 11, 5, and 0.2 μgm^{-3}, respectively. Although this computation may not represent the worst situation, it can be considered as an adverse situation with regard to size of highway, amount of vehicular traffic, and meteorological conditions.

MODEL LIMITATIONS AND CONFIDENCE LIMITS

The application of the Gaussian line source model is restricted to cases where there is horizontal flow and a representative mean wind can be determined between the source and the receptor. The influence of local roughness which is caused by trees or buildings close to the roadway is not included in this model. It is assumed that the surroundings are nearly-level open country. The dispersion parameter values σ_y and σ_z, are basically extrapolations to shorter travel distances of the dispersion parameter values for the Pasquill stability types used in Workbook of Atmospheric Dispersion Estimates (Turner, 1970). Therefore, these may be slightly in error due to local roughness. The initial mixing zone due to the turbulence behind vehicles is estimated from a very limited amount of data and could be subject to change with availability of future field studies. Changing the stability classification by one class will change the concentrations by 10 to 20% close to the source and as much as a factor of 2 at distances greater than about 1 km. Including other sources of error, the accuracy of the model is that estimates might be expected to be within field measurements by a factor of 3 to 5.

There have been some limited comparisons of calculations with the model and field measurements. These comparisons have not been sufficient in number to validate the model with regard to the full range of stability classes or the entire range of possible angles of the wind with the roadway. The initial σ's and the dispersion parameter values themselves are subject to change in response to further field measurements and consideration of local surface roughness. The model should not be applied to highway locations on a fill or built upon elevated columns above the ground surface because in these situations the flow can not be considered horizontal.

MODEL SENSITIVITY

The model assumes concentrations are inversely proportional to wind speed. As mentioned previously, change of stability class will cause considerable changes in concentration. Figure 5 shows the concentrations at receptor locations downwind of the line source for various stability classes for the case of perpendicular winds. A four lane highway 19 meters wide with a 3 meter median was used for this exercise. The highway segment is 5 kilometers long with the receptors perpendicular to the center of the segment. So as to be normalized for the emissions and wind, emissions for each lane were assumed to be 1 g sec^{-1} m^{-1} and wind speed was set at 1 m sec^{-1}. Figure 6 shows the concentrations at receptor locations at the same distances from the identical line source but for wind direction only 10° from the orientation of the line source. Figure 7 shows the change in concentration as the angle of the wind with the source orientation changes for different receptor positions. The same source is used as for Figures 5 and 6. The stability used was class E. Note that for receptors close to the highway, the maximum concentration occurs with small angles of the wind to the source orientation. For receptors at greater distances from the source, the maximum concentration occurs with a larger angle. Although larger, these angles are still quite small, being only 17° from parallel with the line source for a receptor 500 meters from the source.

CONCLUSION

Line source models are useful for estimating concentrations from traffic on highway segments and airport taxiways and runways. A model based on the familiar Gaussian assumptions can be used for the full range of receptor locations and wind orientations with the line source for situations where the wind blows horizontally along the ground surface. These assumptions are most completely fulfilled for at-grade roadways with no significant obstructions to the flow at the side of the road. Although not completely validated for the full range of stability and wind angle situations, sufficient comparisons have been made with field measurements to give some degree of confidence in the use of this model. For more complex highway configurations other approaches such as the use of cellular models are in order.

ACKNOWLEDGEMENTS

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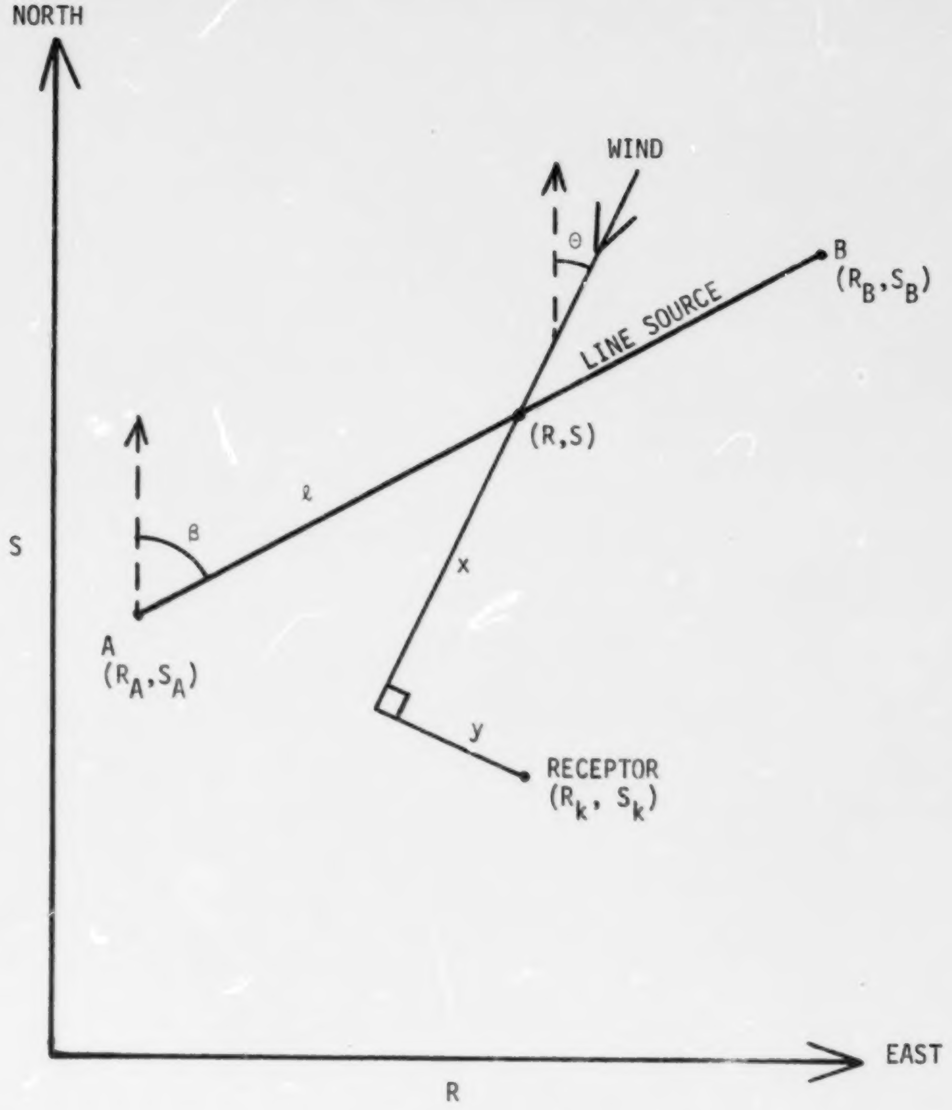
TABLE 1

ONE-HOUR ESTIMATED SUSPENDED PARTICULATE SULFATE AND SULFURIC ACID CONCENTRATIONS IN THE VICINITY OF A BUSY 10-LANE EXPRESSWAY.*

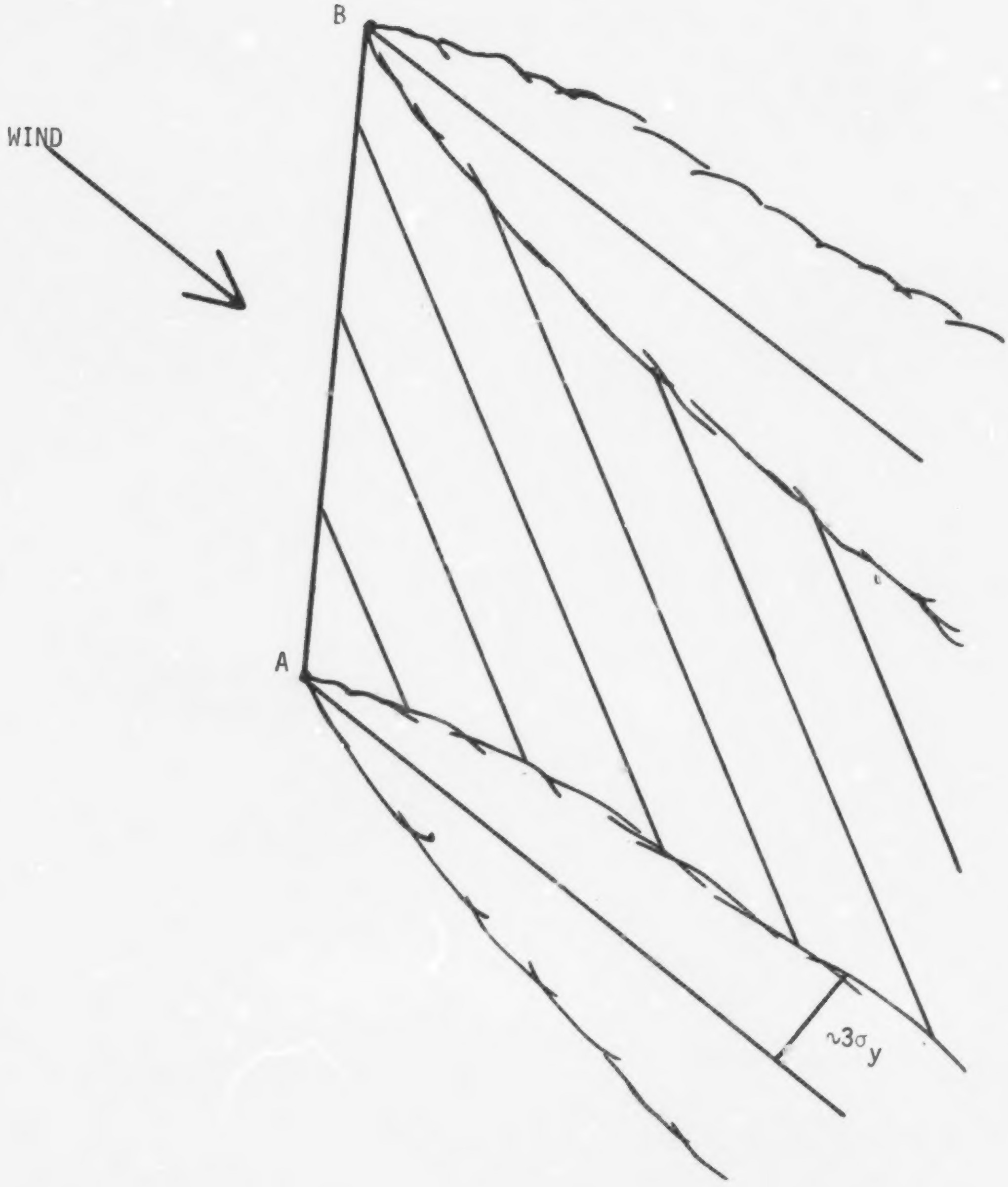
Distance from Edge of Expressway (meters)	Concentration ($\mu g\ m^{-3}$) Normal Meteorology		Adverse Meteorology	
	Wind Perpendicular	Wind at Worst Angle	Wind Perpendicular	Wind at Worst Angle
3	2.1	5	20	88
50	1.3	2	19	33
500	0.3	0.3	5	6

* Assumes 25% of the vehicle miles traveled on a busy 10 lane expressway 2 km long (20,000 vehicles per hour at 30 mi hr^{-1}) are by vehicles equipped with oxidation catalyst devices emitting 0.05 grams of sulfuric acid or sulfate per vehicle mile. Other 75% of vehicle miles emit no sulfuric acid or sulfate.


NORTH
WIND
Θ
B
(R_B, S_B)
LINE SOURCE
(R,S)
ℓ
β
S
x
A
(R_A, S_A)
y
RECEPTOR
(R_k, S_k)
EAST
R

LINE SOURCE AND RECEPTOR RELATIONSHIPS

FIGURE 1


B
WIND
A
~3σ_y

EQUATION (2) CAN BE USED FOR THE AREA WITH LINES BETWEEN THE PLUMES FROM THE END POINTS.

FIGURE 2

ASSUMED INITIAL CONCENTRATION PROFILES IN THE HORIZONTAL AND VERTICAL RESULTING FROM INITIAL σy OF 3, AND INITIAL σz OF 1.5

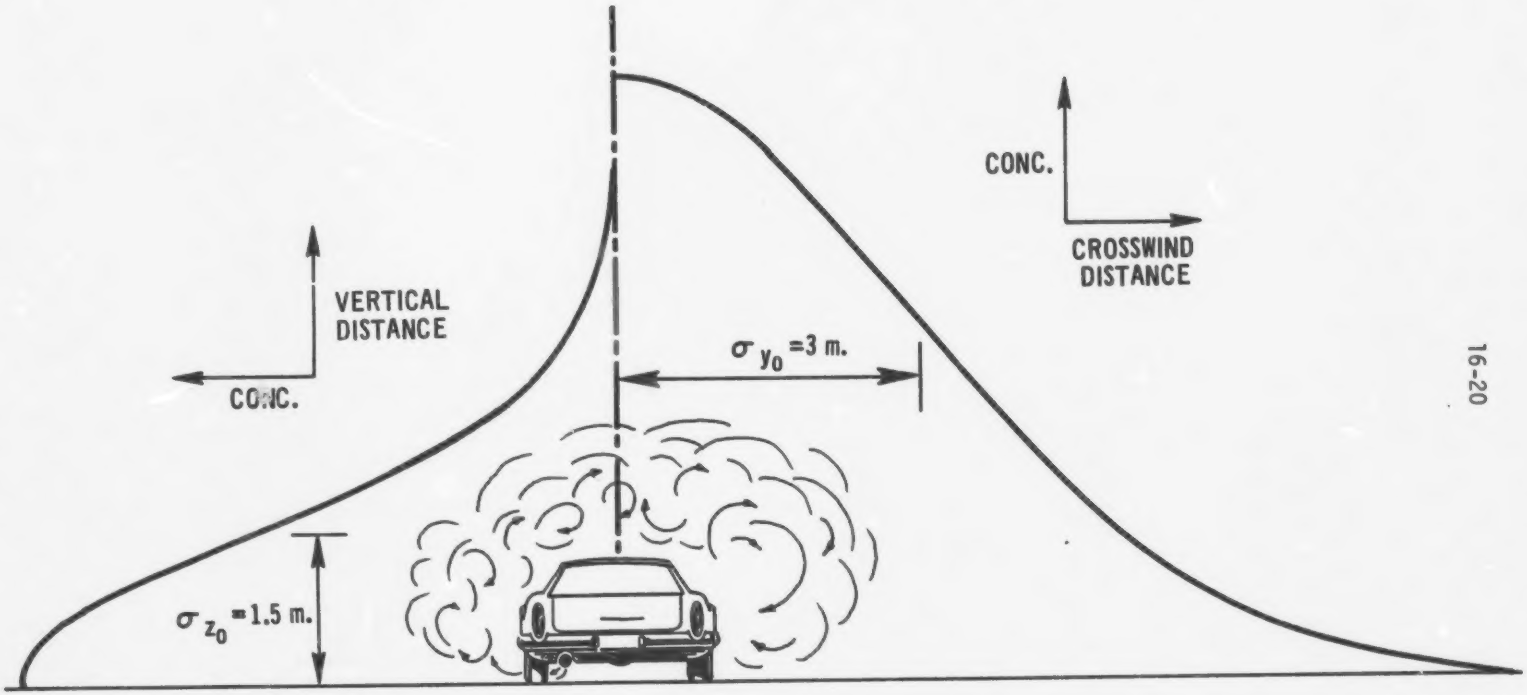

VERTICAL DISTANCE
CONC.
CONC.
CROSSWIND DISTANCE
$\sigma_{y_0} = 3$ m.
$\sigma_{z_0} = 1.5$ m.

FIGURE 3

ESTIMATED HOURLY SULFATE CONCENTRATION VARIATIONS
DURING 24 HOURS AT 3 DISTANCES FROM A HIGHWAY

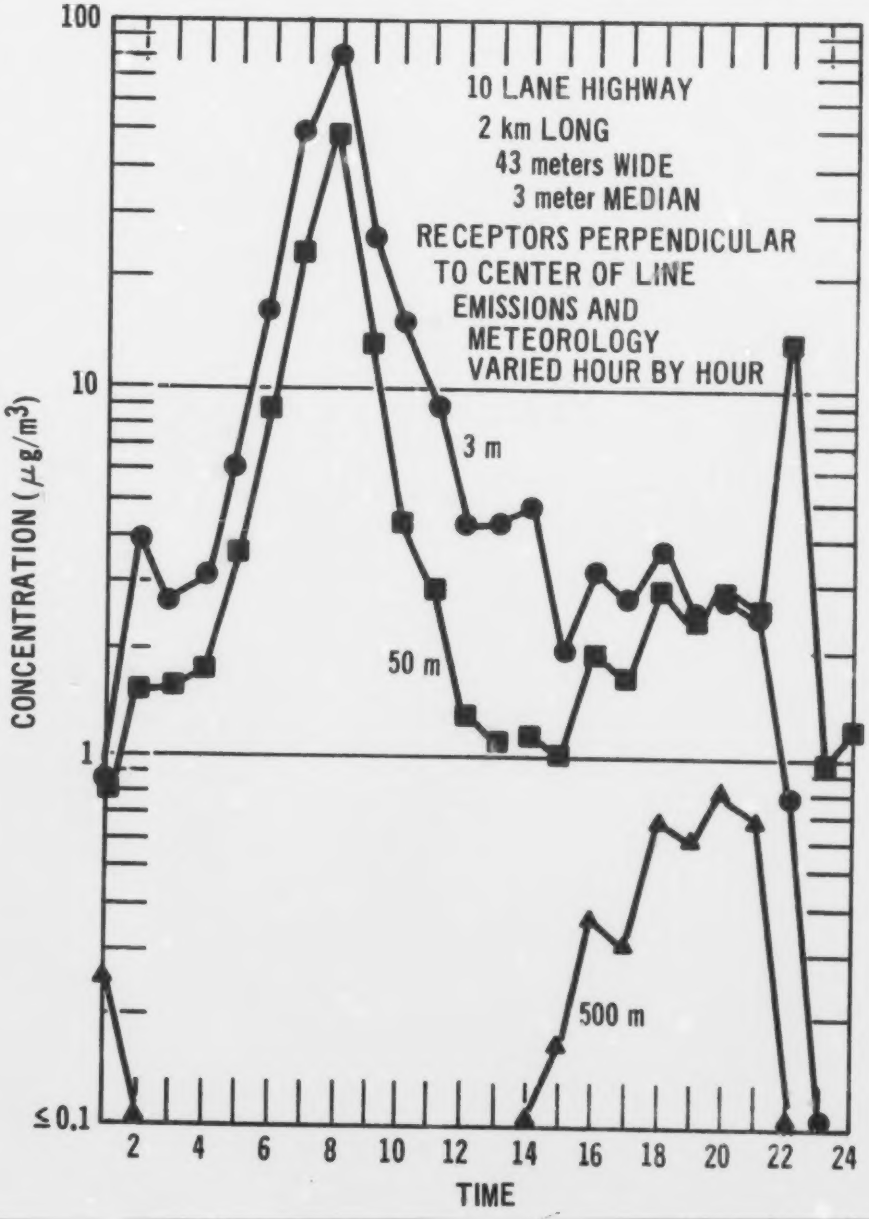


FIGURE 4

X AS A FUNCTION OF DISTANCE FROM ROAD FOR 6 STABILITY CLASSES
(PERPENDICULAR WINDS)

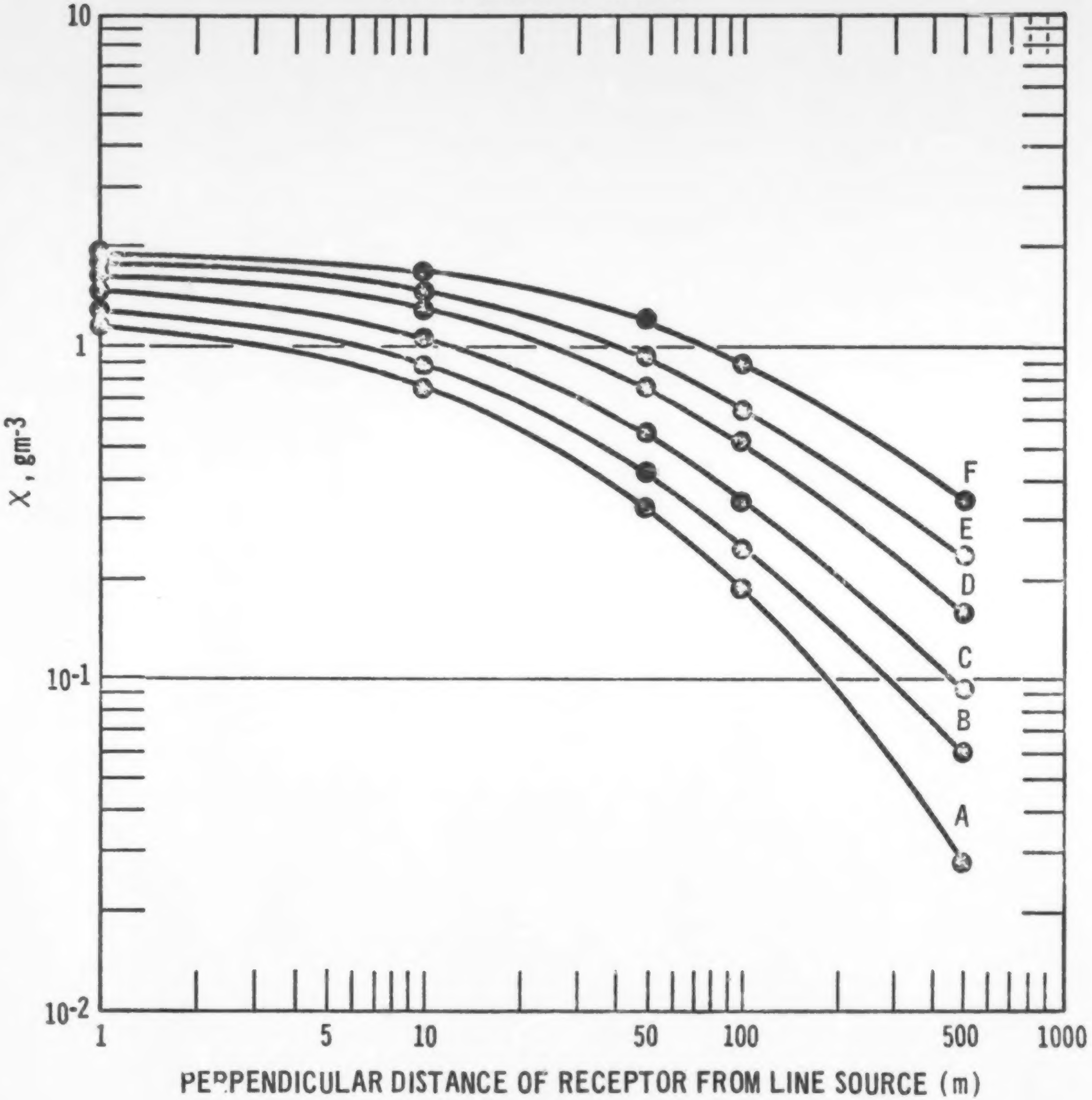


FIGURE 5

X AS A FUNCTION OF DISTANCE FROM ROAD FOR 6 STABILITY CLASSES
(WIND AT ANGLE OF 10° WITH LINE SOURCE)

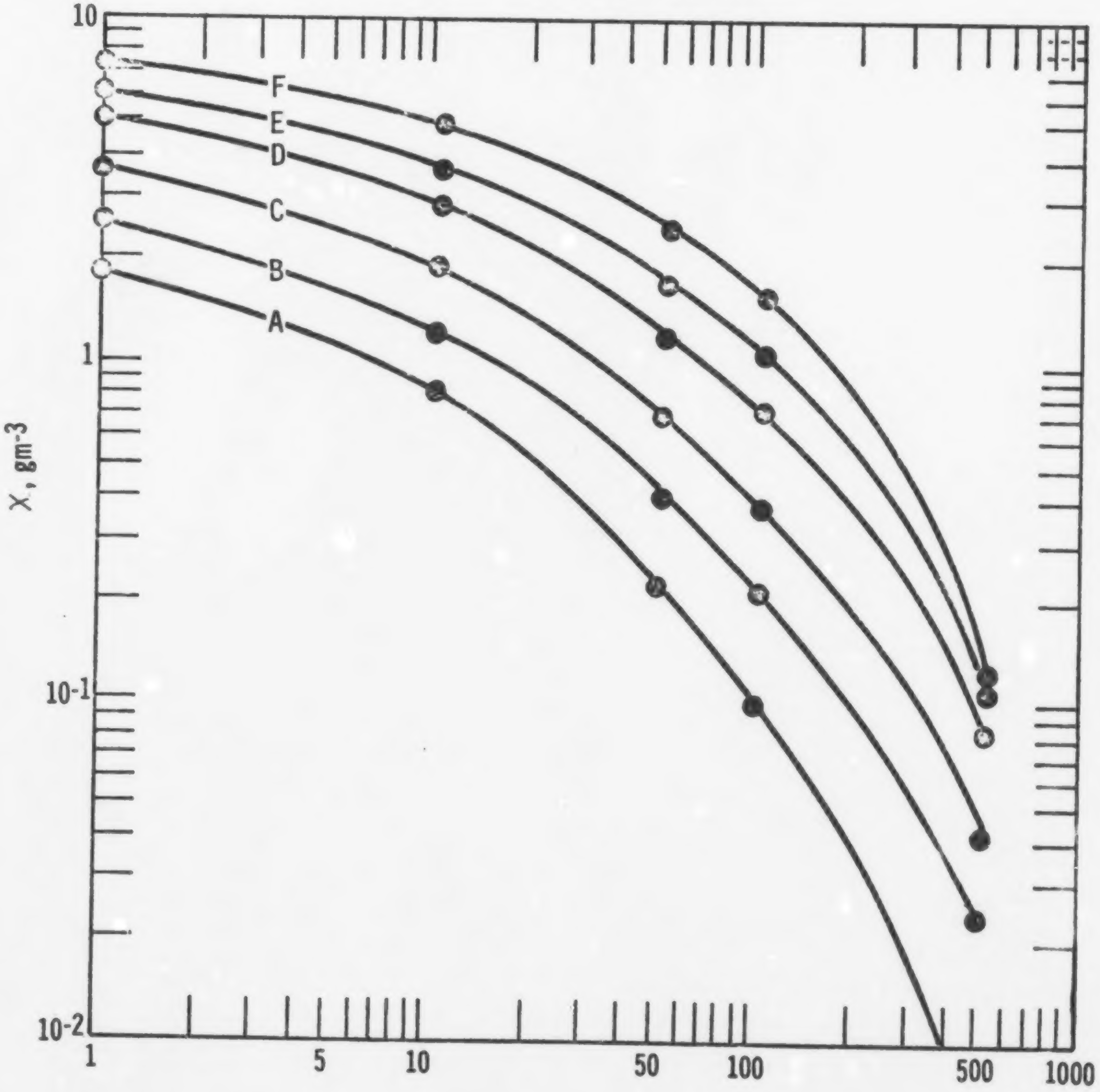


FIGURE 6

χ AS A FUNCTION OF ANGLE OF THE WIND WITH LINE SOURCE
FOR 5 RECEPTOR DISTANCES

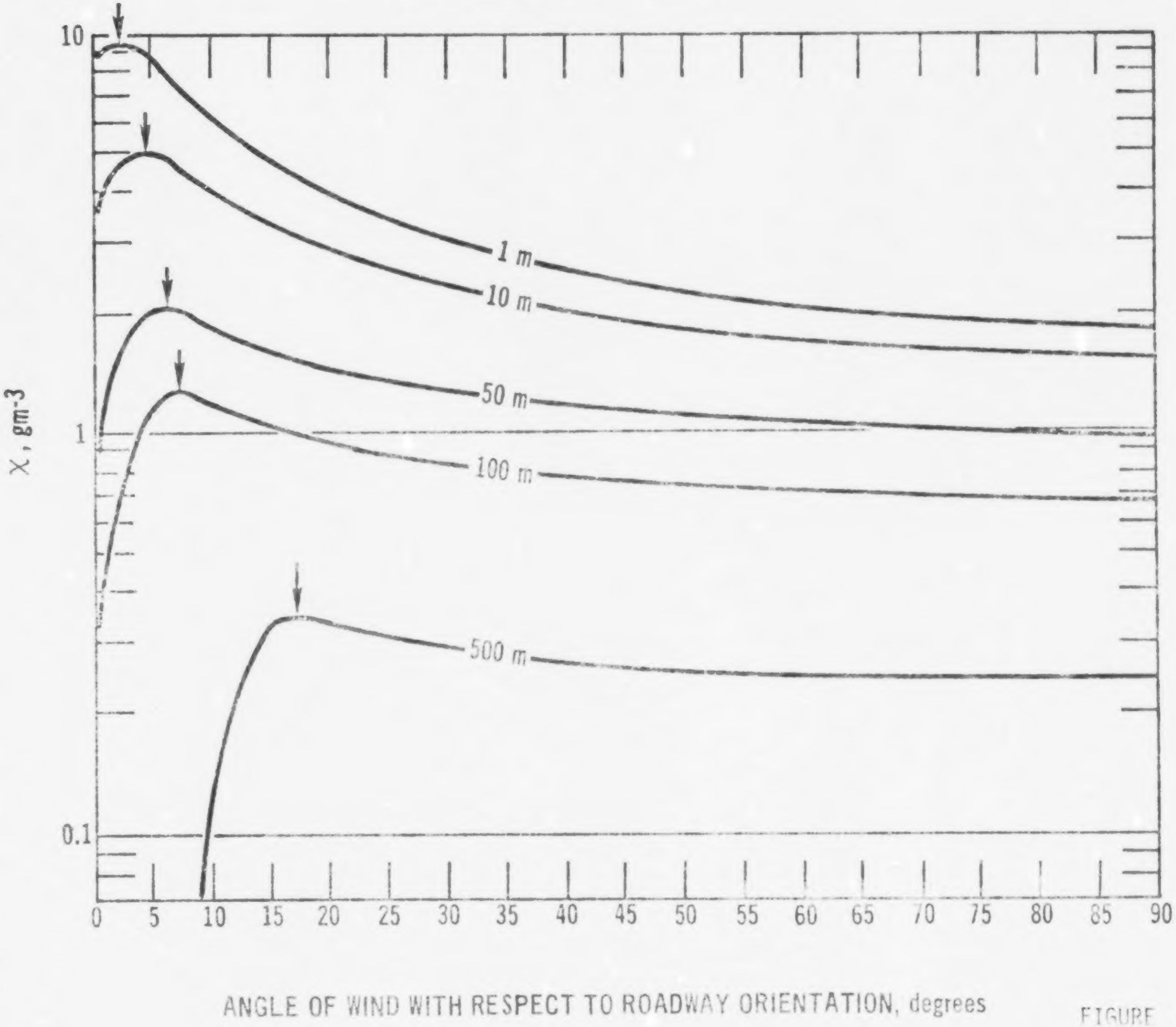


FIGURE 7

Chapter 17

A RATIONAL AIR POLLUTION SURVEILLANCE NETWORK DESIGN

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4-6, June, 1974

1 INTRODUCTION

1.1 Dispersion Modelling: A Management Tool

National and regional air quality management is a complex decision-making process through which policies, laws, and directives to maintain a healthy environment may be developed. Intelligent air management calls on many diversified sciences, such as that of dispersion modelling, for example, to provide extensive, accurate, and current information required to make sound decisions. Because dispersion modelling is only one among the many information tools used in air quality management, it must subject itself to the limits and constraints of the overall project and policies to be administered. To be useful, it must be available when needed and able to relate with all the other tools the manager has at his disposal.

The aim of this paper is to illustrate the application of dispersion modelling in one air quality management task - that of designing air pollution surveillance networks. All aspects of the design, including those not related to dispersion modelling, are purposely described to show the role of modelling in such a project and its interaction with the overall project.

1.2 General Concepts of Network Design

The establishment of national or regional surveillance networks is a relatively recent task for most air pollution control agencies. The late sixties and especially the seventies have seen an extremely rapid growth of air pollution monitoring in the developed areas of the world. In some cases existing regional networks were expanded by the addition of new stations and new equipment. In other cases new networks were established. This process of expanding and improving networks is a continuing one. Monitoring equipment is changing and at the same time more reliable monitors are coming into the market.

The task of designing efficient monitoring networks on a regional or national scale is not yet over. In the past this task was carried out rather intuitively, based on limited observation, personal judgement, and often times plain expediency in an effort to get something going. With the increased preoccupation with air pollution, more public funds suddenly became available and networks had to be set up quickly. At the same time development of effective air pollution control management tools was just starting, especially the emission inventory and the multiple source diffusion model.

Today, however, these tools should be sufficiently developed and tested. It is time that they be passed on from the development area to the management area where they can be valuable aids in making rational and efficient decisions. The application of such tools to the design of efficient surveillance networks is thus now not only feasible but also mandatory.

2 PURPOSE FOR SURVEILLANCE

Air sampling equipment is set up essentially to assess the air quality in the immediate vicinity of the monitor. The measurement of air quality, however, is done for one purpose only, to serve as a basis for decision making. Air pollution monitoring is, therefore, not an end in itself but only one tool among others in the hands of the decision maker . According to the control actions envisaged, the reasons for establishing surveillance networks are as follows:

(a) long-term surveillance

(i) to monitor air quality in areas where it is already satisfactory, so that any deterioration may be detected and control measures applied as soon as possible;

(ii) to quantify improvements required in areas where air quality is unsatisfactory and thus indicate the type and degree of control required;

(iii) to evaluate the effectiveness of control measures implemented in an area and to follow the improvements with time;

(iv) to provide an alarm for real-time control systems in the case of emergency episodes.

(b) short-term surveillance (temporary stations)

(i) to determine air quality in areas in need of intensive control measures or affected by rapid development, to plan long-term surveillance or control strategies;

(ii) to provide data for specific research projects - the validation of diffusion models would fall in this category.

3 NETWORK DESIGN

When designing a surveillance network, its purpose should be kept in mind; hopefully the result will be an efficient network that will provide reliable data to the decision maker. We will concern outselves here with the design for long-term surveillance networks only, although many of the principles set forth will be equally applicable to short-term surveillance network design. The stages in network design may be stated as follows:

(a) Identify areas in need of surveillance by use of guidelines, in response to complaints or requests, or by any other means.

(b) Identify the pollutants present and thus the type and number of monitors to be installed.

(c) Determine the general locations where these monitoring stations are to be located keeping in mind the aim of the monitoring program.

(d) Determine the actual location of the monitors according to physical constraints such as power availability, access ease, security, and absence of interferences.

(e) Select and design the actual equipment installations with all supporting hardware and plan the construction of these installations.

(f) Establish operating and maintenance procedures and responsibilities.

(g) Establish data collection, handling, and reporting procedures and responsibilities.

(h) Evaluate the overall network design after a reasonable trial period, and implement appropriate revisions of the network as required.

4 A RATIONAL DESIGN PROCEDURE

The design stages set forth above are the basis for a rational design procedure. In the past these steps were occasionally performed in reverse order, often cutting corners intuitively. A rational design procedure would cover these stages step by step using the best available management tools while remaining within certain time limits.

4.1 Identify Need

Prior observations may serve to establish Surveillance needs. As is often the case, however, these observations are either limited or made with simple equipment. In many cases no prior observations are available. A guideline based on area population and existing pollution level as suggested by the United States Environmental Protection Agency (1) may be used to identify need.

The best tool in this respect, however, is the emission inventory. Firstly, it provides a base for comparing different areas by standardizing the compilation procedure. Secondly, it is a prerequisite for setting up a reliable diffusion model. The types and quantities of pollutants emitted in the area are first identified by the emission inventory. The gross pollutant emission may then be combined with the overall demographic and meteorological parameters in the simple box diffusion model as suggested by Gifford and Hanna (2):

$$X = C \frac{Q}{U}$$

Where X - Pollutant concentration (g/m^3)

C - Constant

Q - Pollutant area emission ($g/m^2 . s$)

U - Average wind speed (m/s)

Thus general guidelines may be set up based on one simple estimation which has been shown to be quite reliable for this purpose (3).

4.2 Identify General Locations

The aim of monitoring is to measure pollution. Monitoring stations in a given area should therefore be established where the heaviest pollution occurs.

To identify these locations, a dispersion model may be used. If an emission inventory has been compiled, half of the work of producing the model has already been done.

There are presently available a number of multiple-source models that are ideal for determining long-term pollution patterns (3). These models have been shown to be reliable enough for the purpose of network design and are suited to the use of approximative data input. Thus the use of the ATDL, AQDM, or variations thereof can be used for intelligent selection of sites.

4.3 Identify Specific Location

Choosing a specific site for placing the monitoring equipment is a task that must be done locally. Having chosen the general area wherein to locate a station, a field search is necessary to find an appropriate site. The specific site requirements are many: local meteorological conditions on the microscale, proximity of neighbouring sources, engineering and social conditions, and others. The sampling site must be located where air samples that are representative of the area for which air quality measurements are desired may be obtained.

4.4 Hardward Design

Having decided (a) what pollutants to measure, and (b) where to sample, the monitoring station may be laid out. First, a decision must be made concerning the specific instruments to be used. This decision will be made on the basis of instrument sensitivity, accuracy, reliability, and maintenance need. Instrument evaluation is thus also a necessary requirement to rational surveillance network design.

Second, after an instrument has been chosen, the overall station design can proceed. Included in this design, besides the usual considerations of access, power, services, and safety, will be a design for a proper air sampling system. Proper sampling procedures complement proper site selection. Sampling system design includes such factors as location of the air intake in respect of the ground and surrounding buildings, as well as the design of the piping through which the sample will be carried. Just as a specific site should provide air samples that are representative of the air mass of an area, a sampling system should provide the instrument with air samples that are indeed representative of the air surrounding the site.

4.5 Operating Procedures

Good operating procedures must complement good monitoring station design. From the start operating procedures should be laid down to maintain effective air quality measurement.

To be determined before a station is operational are

(a) maintenance requirements, schedule, and responsibility; and

(b) calibration requirements, schedule, and responsibility.

Finally, assuming all previous steps were followed and valid representative measurements of air quality are made, the information must be passed on to management. The information must be passed on in a format which is understandable and complete. Thus, data collection, reduction, and compilation procedures must also be established.

4.6 Design Evaluation

After a particular network or station has been in operation for some time, it should be evaluated as to the effectiveness of the design. The sampling and measurement design and hardware should be evaluated at this time.

5 THE ROLE OF MODELLING AND ITS CONSTRAINTS IN NETWORK DESIGN

Diffusion models are used in the design of surveillance networks strictly as a tool. As such it must subject itself to the overall aims of the design project and work within the project constraints. The primary constraint is one of time. A deadline is usually set for completion of a surveillance network. This restriction limits the time which can be spent in obtaining an emission inventory if none is available. Of necessity then, the emission inventory will often be only an estimate, although a fairly reliable one. As concentration estimates obtained from a dispersion model are directly proportional to the level of emissions, applying an extremely sophisticated dispersion model to approximate data serves no useful purpose. Time limits, also, would not permit one to obtain detailed meterological data for input to the model. The constraints under which the model will operate are summarized as follows:

(a) maximum time limit during which a model will have to be produced;

(b) minimum of meteorological input data (usually only a wind rose from nearby airport);

(c) minimum emission data (some fairly accurate data for large sources with estimated data for remaining sources).

The model required in this application is therefore a simple one that can meet project constraints. The situation in this case is either to provide a model which will operate within the limits or omit modelling altogether from the design procedure. Fortunately, long-term climatological models have been shown to operate well within these constraints. For surveillance design needs, long-term concentration estimates are usually quite sufficient.

6 FUTURE REQUIREMENTS

The applicability of these modelling tools to the design of air pollution surveillance networks is valid only for monitoring sulphur oxides and suspended particulates. The case of the automotive and photochemical pollutants is substantially different. For automotive pollutants, the diffusion scale is much smaller and the overall diffusion and wind patterns are much more complex. For photochemical pollutants a chemical reaction term must be added to the transport term. Not only does the addition of such a term complicate calculations, but rate constants can be expected to change with different geographical areas and with the season.

7 CONCLUSIONS

The rational design of air pollution surveillance network is possible with the help of two basic and complementary tools: the emission inventory and the dispersion model. Simple climatological models are capable of providing reliable information for the design of networks and can operate within the constraints of such a network design project. This statement applies only for pollution by SO_2 and particulates. For these pollutants it is suggested that the use of these models now be implemented. Research should be directed to the development of similar simple models for dispersion of automotive and photochemical pollutants. A real need exists in this area.

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Chapter 18

APPLICATION OF THE AQDM MODEL AND THE ATDL MODEL AND COMPARISON OF THE RESULTS

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

Application of the AQDM Model and the ATDL Model and Comparison of the Results

by

J. Strott, A. Braig and K. Michelmann

1. Introductory Remarks

A number of mathematical models are available for computing the annual mean of the ground-level concentration resulting from air pollution. Aa most of these models were tested in and applied to areas in the U.S.A., it seemed necessary to evaluate such a model for European meteorological conditions. Another goal was to check the differences between the so-called "sophisticated" and "simple" models.

Variations of the AQDM model /6/ and the ATDL model /2/ were tested and applied to the Frankfurt area.

2. Test of the Air Quality Dispersion Model (AQDM)

The original version of the AQDM as described in /6/ uses stability classes after Turner, a plume rise formula by Holland and Slümke and a special definition of mixing depths by Tikvart and Martin /5/ which allows over cities only the neutral stability class with a mixing depth of 100 m (Table 1). In order to check the influence of these parameters, four different versions were tested using the input data for Test City /6/.

The following table shows the result of this sensitivity analysis.

Criterion	Variation 1	Variation 2	Variation 3	Variation 4	Variation 5 *
Plume rise formula	Holland-Stümke	Briggs	Holland-Stümke	Briggs	Briggs
Mixing depth	Tikvart-Martin	Tikvart-Martin	Klug	Klug	Klug
Slope of the regression line	.47	.72	.49	.73	.80
Correlation coefficient	.99	.96	.96	.89	.99

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*) Variation 5 is identical with Variation 4. The difference in the slopes of the regression lines and the correlation coefficient result in the exemption of receptor No. 3 of Test City

Table 1: Tested variations of the AQDM

The mixing depths were as follows:

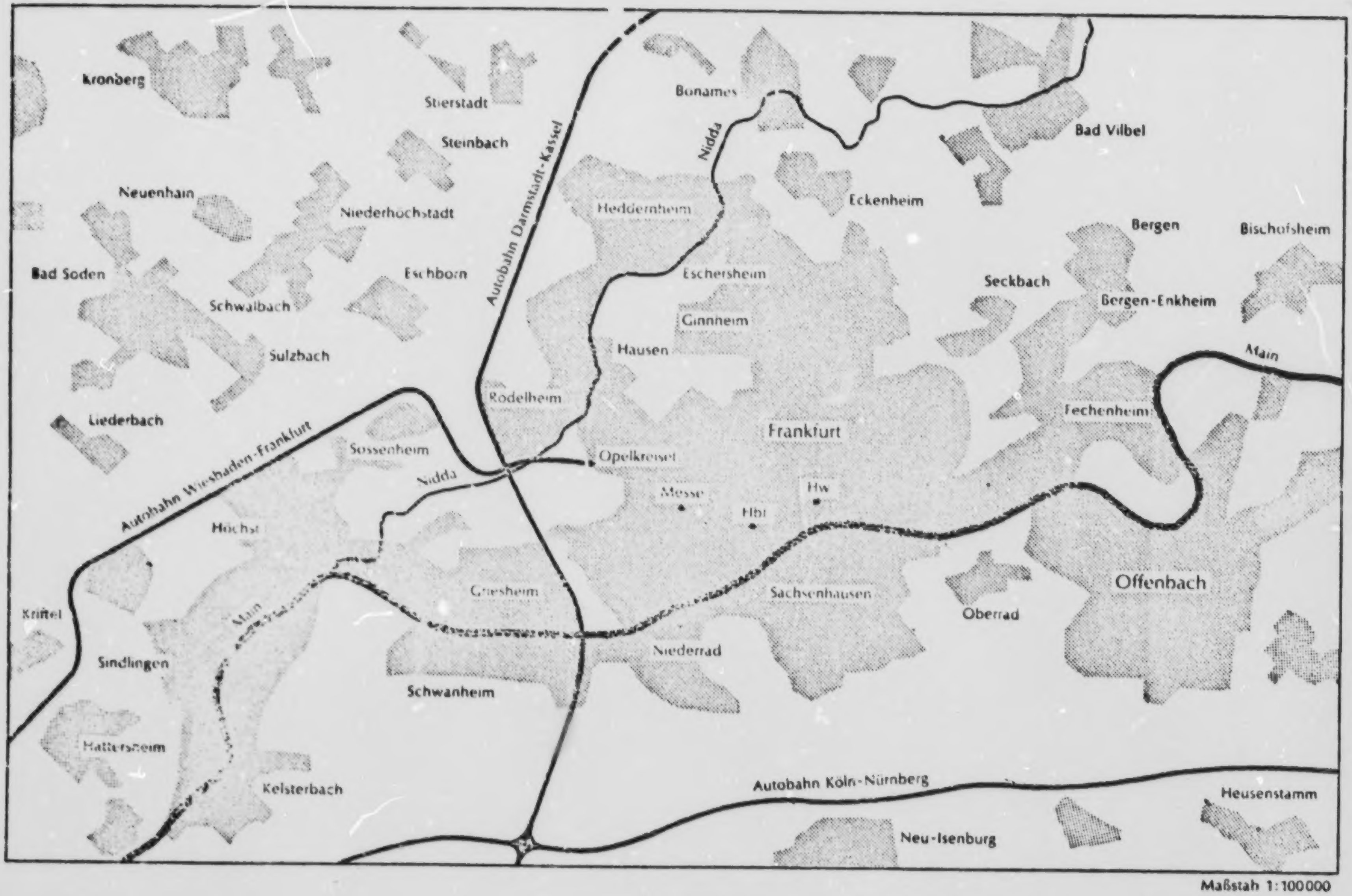
Stability class (Klug)	Mixing depth (m)	
	Tikvart	Klug
I	1000 (day) 550 (night)	0
II		0
III_1	1000	1200
III_2	1000	1200
IV	1500	1500
V		1800
III_1	100 over cities	no exception

Table 2: Mixing depths

3. Application of the AQDM to Frankfurt

The AQDM was applied to an area of 10 km x 19 km which includes the City of Frankfurt (Fig. 1).
As input data an emission inventory of 1971 /5/ was used which is based on a grid of 500 x 500 m.
All emissions from point sources emitting less than 5 kg SO_2/h were added to area sources. Thus we had only 46 point sources (Fig. 1 appendix) with emissions of more than 5 kg SO_2/h and 210 area sources (Fig. 2 appendix) with an emission height between 10 m and 24 m. In order to get a reasonable background concentration, a stripe of 4 km width was laid around the boundary of the research area. As these area sources had a size of 4 km x 4 km, another 17 area sources had to be added.

The total emissions amounted to 45,500 t/year, 27,000 t of which came from industrial sources and 7,500 t were background emission. The 46 point sources included all the major sources within 12 km from the boundary of the research area.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Stierstadt
Steinbach
Bonames
Bad Vilbel
Neuenhain
Niederhöchstadt
Nidda
Heddernheim
Eckenheim
Bergen
Bischofsheim
Bad Soden
Eschborn
Autobahn Darmstadt-Kassel
Eschersheim
Seckbach
Bergen-Enkheim
Schwalbach
Ginnheim
Sulzbach
Hausen
Main
Rödelheim
Fechenheim
Liederbach
Frankfurt
Sossenheim
Opelkreisel
Nidda
Messe
Hw
Autobahn Wiesbaden-Frankfurt
Hbf
Höchst
Offenbach
Griesheim
Sachsenhausen
Main
Kriftel
Oberrad
Niederrad
Sindlingen
Schwanheim
Hattersheim
Kelsterbach
Autobahn Köln-Nürnberg
Heusenstamm
Neu-Isenburg
Maßstab 1:100000

Fig. 1: Sketch of the research area (City of Frankfurt and surroundings)

The meteorological input was derived from the statistics of the Rhein-Main Airport from 1955 to 1966.
On the basis of these data, Variation 4 of AQDM was used with the following windspeed classes and dispersion parameters ($\sigma_z = a\,x^b$)

Class	Windspeed (kn)	Mean windspeed (m/s)
1	0 - 2	1.0
2	3 - 5	2.1
3	6 - 8	3.6
4	9 - 12	5.3
5	13 - 17	7.5
6	18 - 30	10.2

Table 3: Windspeed classes

Stability class (Klug)	a	b
I	0.11727	0.67
II	0.14856	0.73
III_1	0.19943	0.76
III_2	0.22294	0.80
IV+V	0.27937	0.90

Table 4: Coefficients for dispersion parameters after Pasquill

The results of this computation are shown as isopleths in Fig. 2; they are validated in Fig. 3 (appendix) and Fig. 4 (appendix). Comparison of the results shows that the deviation of the two series of observations is of the same order as the deviation of the calculated values from the observed ones (about 20 %). An extra computation showed that area sources within four kilometers of a receptor contribute about 75 percent to the ground-level concentration, while the influence of higher ($H > 100$ m) point sources extends to a much larger range. It was calculated that a point source emitting 54 kg SO_2/h of a distance of 16 km from a receptor still contributed 1 percent to the ground-level concentration of the receptor in the center of Frankfurt.

4. Modification of the AQDM

To obtain information about the influence of other plume rise formulas and dispersion parameters, another modification of AQDM was calculated.

Using the same emission inventory and meteorological data as input, the plume rise formula of Moses and Carson for the neutral stability class was inserted, the dispersion parameters of Singer and Smith ($\sigma_z = a\, x^b$) being applied. In addition, the wind profile was varied with the effective height of the stacks:

$$\bar{u} = \frac{\bar{U}(z_o)}{m+1} \left(\frac{h}{z_o} \right)^m \; ; \quad h \geq 10 \text{ m.}$$

Stability classes Klug	Turner	a	b	m
IV, V	2	1.42	0.745	0.10
III_2	3	1.26	0.169	0.22
III_1	4	1.13	1.070	0.28
I, II	5	0.992	1.010	0.40

Table 5: Coefficients of dispersion parameters according to Singer and Smith and wind-profile parameters

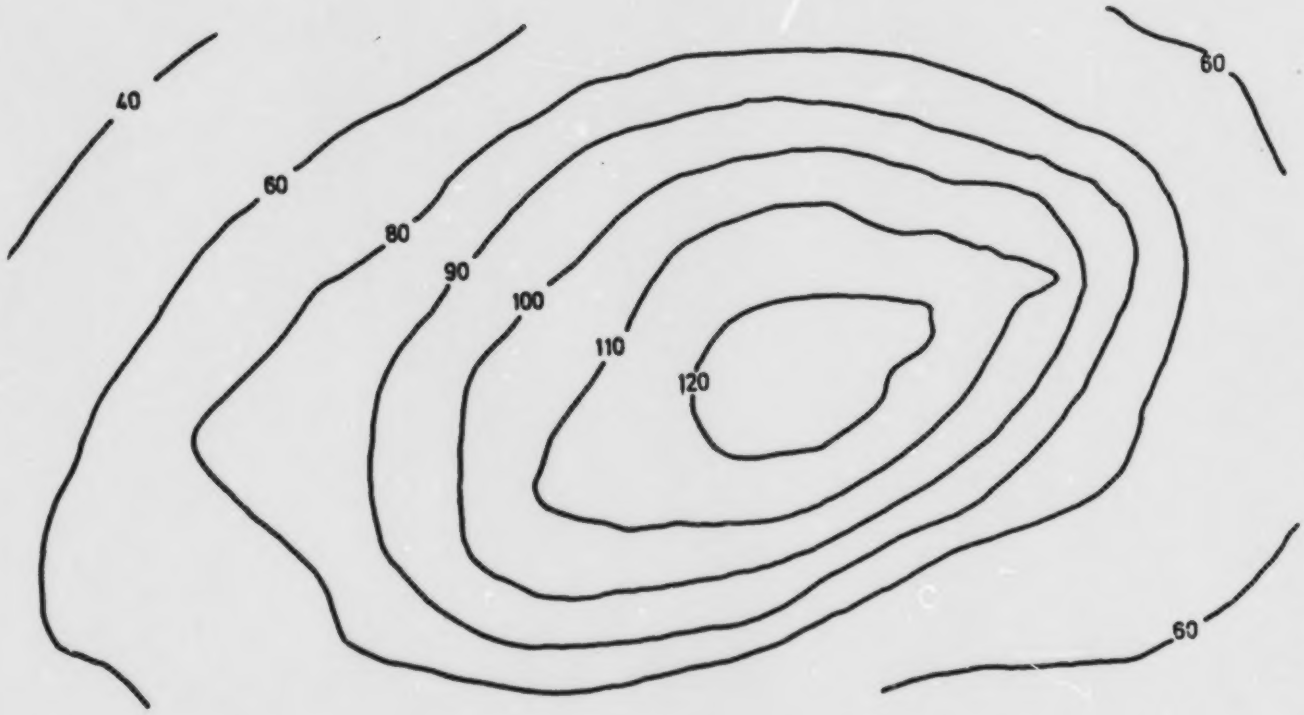
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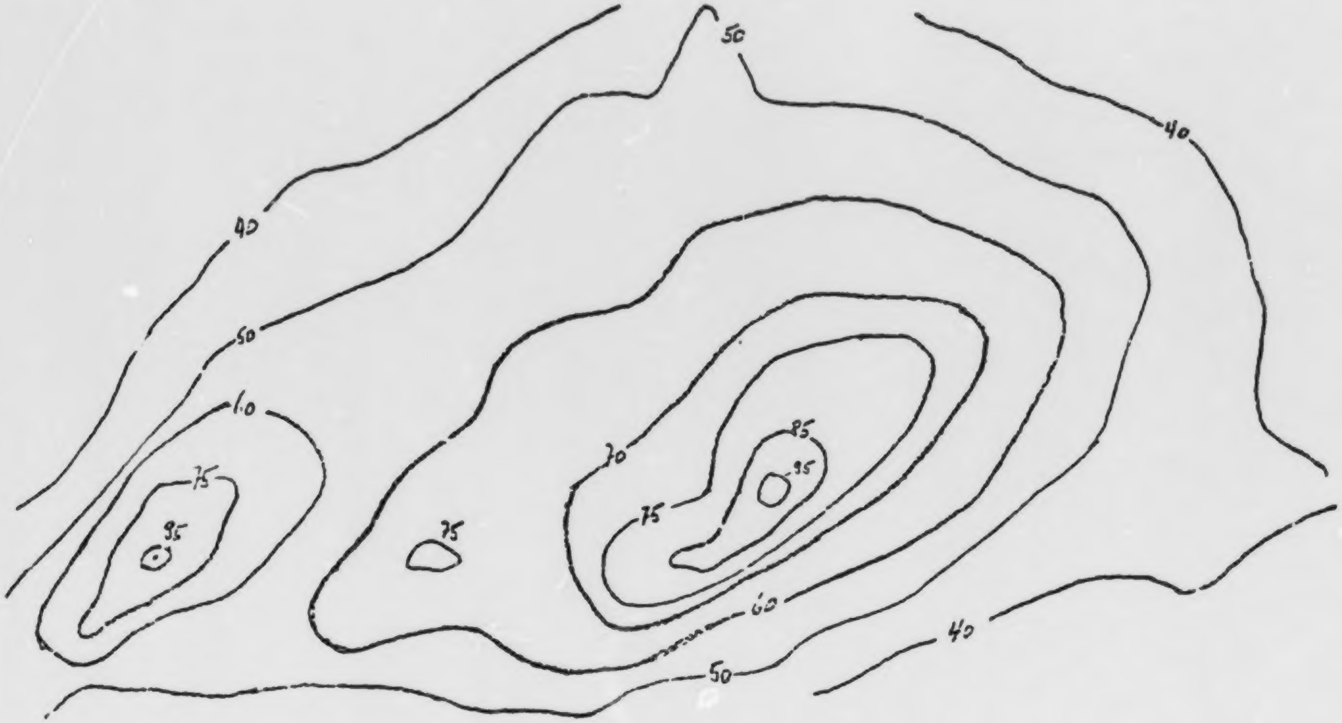
Fig. 2: Isopleths of annual mean concentration of SO_2 ($\mu g/m^3$) calculated with AQDM, 1st application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60
40
50

Fig. 3: Isopleths of annual mean concentration of SO_2 (ug/m^3) calculated with AQDM, 2nd application

The results of this modified version are shown as isopleths in Fig. 3 and compared with observations in Fig. 5 (appendix).

It is readily seen that the concentrations are underestimated though the shape of the isopleths is similar to the first calculation. The main difference in shape is a local maximum in the Southwest of the research area. Considering that the Singer-Smith dispersion parameters are thought to be used for higher sources ($H > 100$ m), this result is not surprising. A rough estimate showed that a combination of these parameters with Pasquill parameters for area sources would have given about the same concentrations as in the first calculation.

5. Application of the ATDL Model to Frankfurt

The ATDL Model is a so-called "simple" model, which means that it is easy to apply although the theoretical background is highly sophisticated. To obtain comparable results, the same input data were used as in the case of the AQDM. This again required a grid as small as 1 km. The effective height of the 46 point sources was precalculated using the Briggs plume rise formula and classified by height classes differing by 10 m. As the ATDL model allows only one windspeed per stability class, we used mean windspeeds of 1.13, 1.7, 5.5, 3.2 and 2 m/s for the stability classes I to IV after Klug and the dispersion parameters of Table 3.

Two different calculations were made. In the first version the model was calculated four times, each time with a different stability class, a percentage due to the frequency distribution being used for the AQDM and the concentrations were summed up for every receptor. In the second version, the results of which are shown in Fig. 4, only stability class III_1 with a mean windspeed of 3.2 m/s was used. In both versions the wind direction distribution was the same.

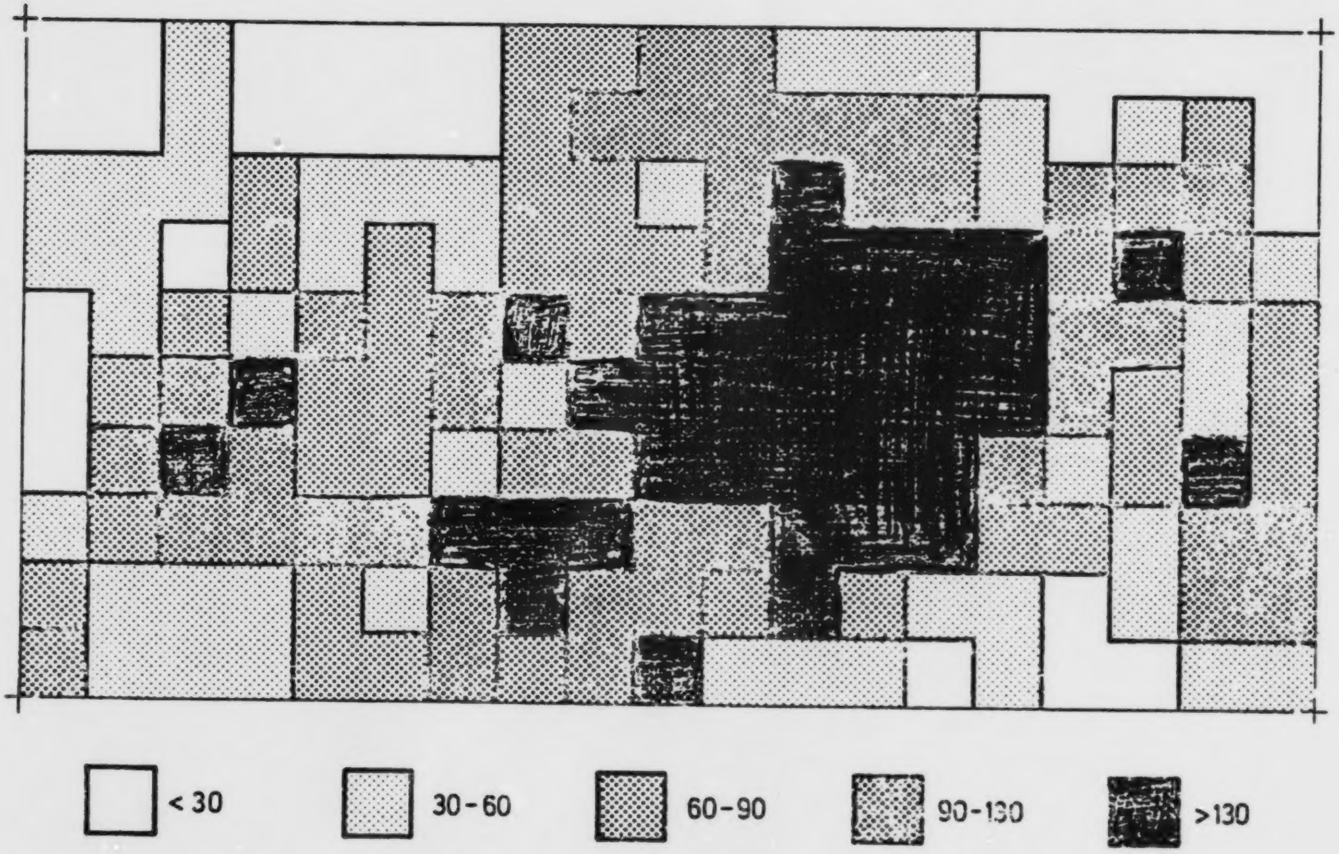
< 30
30-60
60-90
90-130
>130

Fig. 4: Annual mean concentration of SO_2 ($\mu g/m^3$) calculated with the ATDL model

As the ATDL model allows the ground-level concentration to be calculated for each receptor only from sources not farther away than 4.5 grid widths (i.e. 81 surrounding meshes), an undercalculation of the concentrations was expected. But both versions gave an overestimate of the concentration in the center of Frankfurt (highest value 782 $/ug/m^3$ in version 1 and 442 $/ug/m^3$ in version 2 instead of 126 $/ug/m^3$ and an underestimate at the outskirts. A detailed comparison shows that the calculated concentrations exactly reflect the emission inventory for area sources (cf. Fig. 4 and Fig. 2 appendix).

It seems that the results could be bettered if it were possible to calculate the area sources of a height greater than zero and if a sectoral wind rose were used instead of the present wind-direction distribution. In addition, a three-dimensional frequency distribution of meteorological parameters should be used (i.e. different wind speeds for the individual stability classes), and all point sources should be able to contribute to every receptor.

6. Conclusions

The AQDM gives a fairly good estimate of the ground-level concentration, while the results of the ATDL model are unreliable with the grid width used. Since the computation time for the ATDL model is by a factor of 20 less than the computation time for the AQDM, the ATDL model should be modified in the above-described way for smaller grids and used for rough estimates. The unmodified ATDL model can only be used with larger grids (5 km grid width) for surveay of air pollution in large regions.

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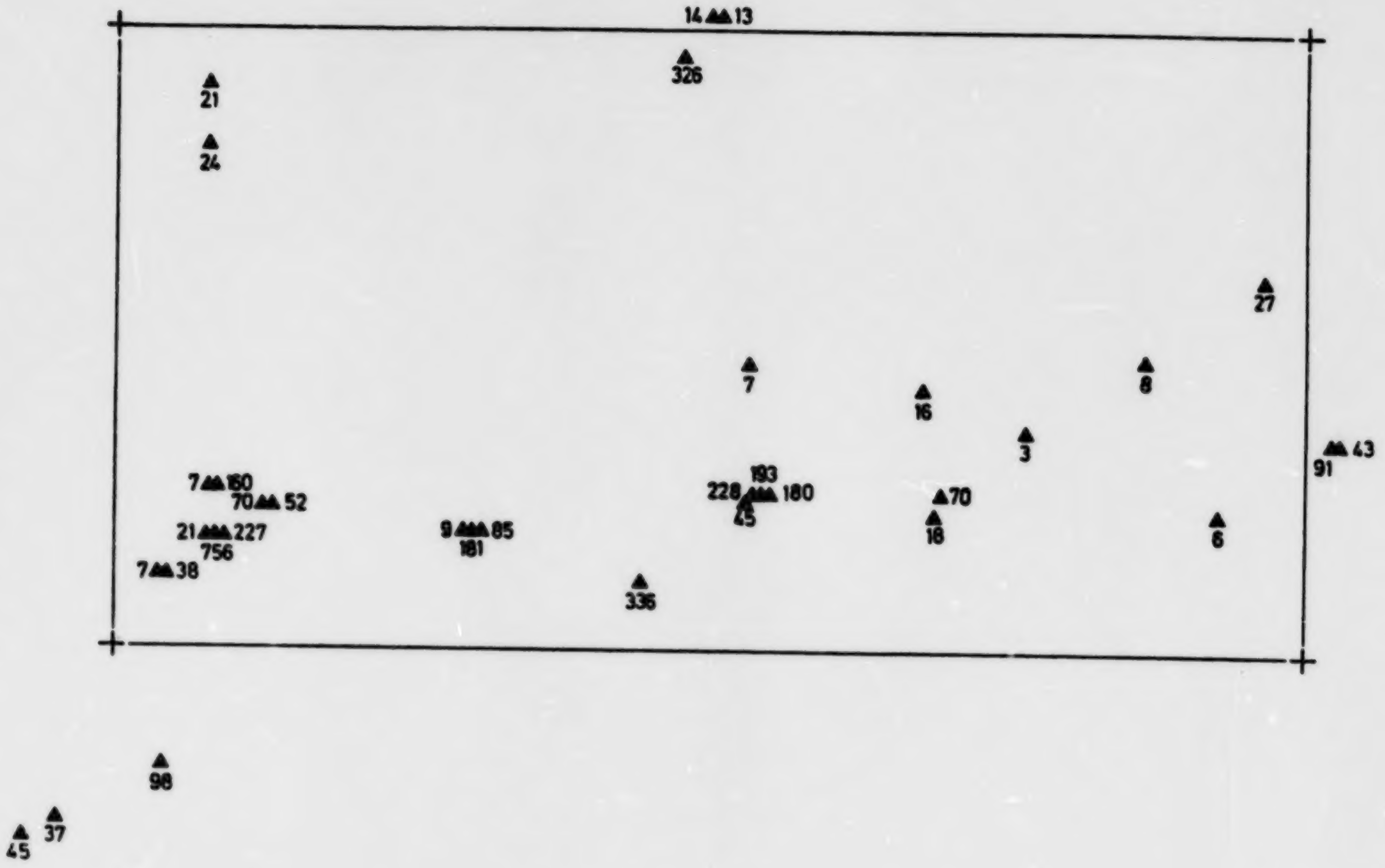
APPENDIX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7 160
70 52
193
228 180
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756
9 85
181
7 38
336
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45
37

Fig. 1: Point-source~~s~~ distribution in the Frankfurt area ($kg\ SO_2/h$)

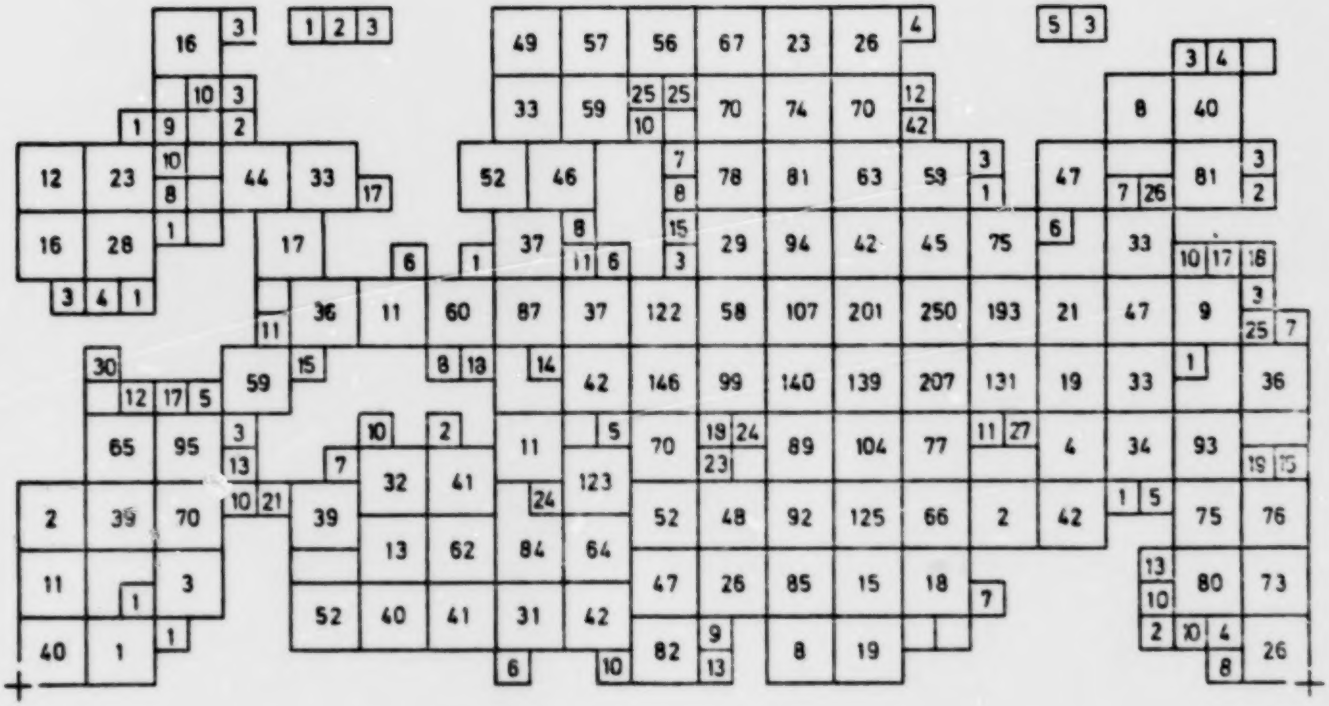
16 3 1 2 3 49 57 56 67 23 26 4 5 3
3 4
10 3 33 59 25 25 70 74 70 12 8 40
1 9 2 10 42
12 23 10 44 33 17 52 46 7 78 81 63 59 3 47 81 3
8 8 1 7 26 2
16 28 1 17 6 1 37 8 11 6 15 3 29 94 42 45 75 6 33 10 17 16
3 4 1
36 11 60 87 37 122 58 107 201 250 193 21 47 9 3
11 25 7
30 12 17 5 59 15 8 13 14 42 146 99 140 139 207 131 19 33 1 36
65 95 3 10 2 11 5 70 19 24 89 104 77 11 27 4 34 93
13 7 23 19 15
32 41 123
2 39 70 10 21 39 24 52 48 92 125 66 2 42 1 5 75 76
13 62 84 64
11 1 3 47 26 85 15 18 7 13 80 73
10
52 40 41 31 42
40 1 1 82 9 8 19 2 10 4 26
6 10 13 8

Fig. 2: Area-source distribution in the Frankfurt area (kg SO_2/h)

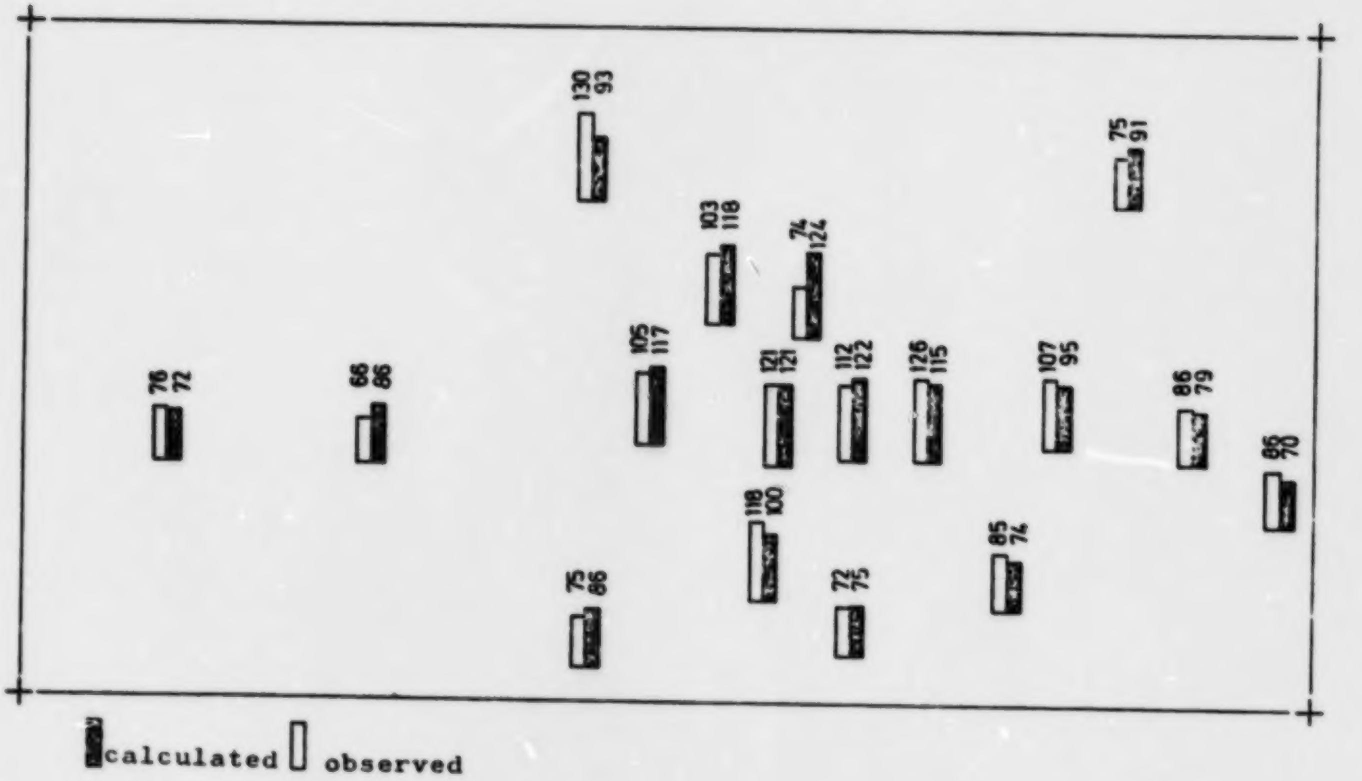

Fig. 3: Comparison of observed and calculated (AQDM, 1) annual mean concentrations ($\mu g/m^3$). Measurements made by Institut für Wasser-, Boden- und Lufthygiene, Berlin

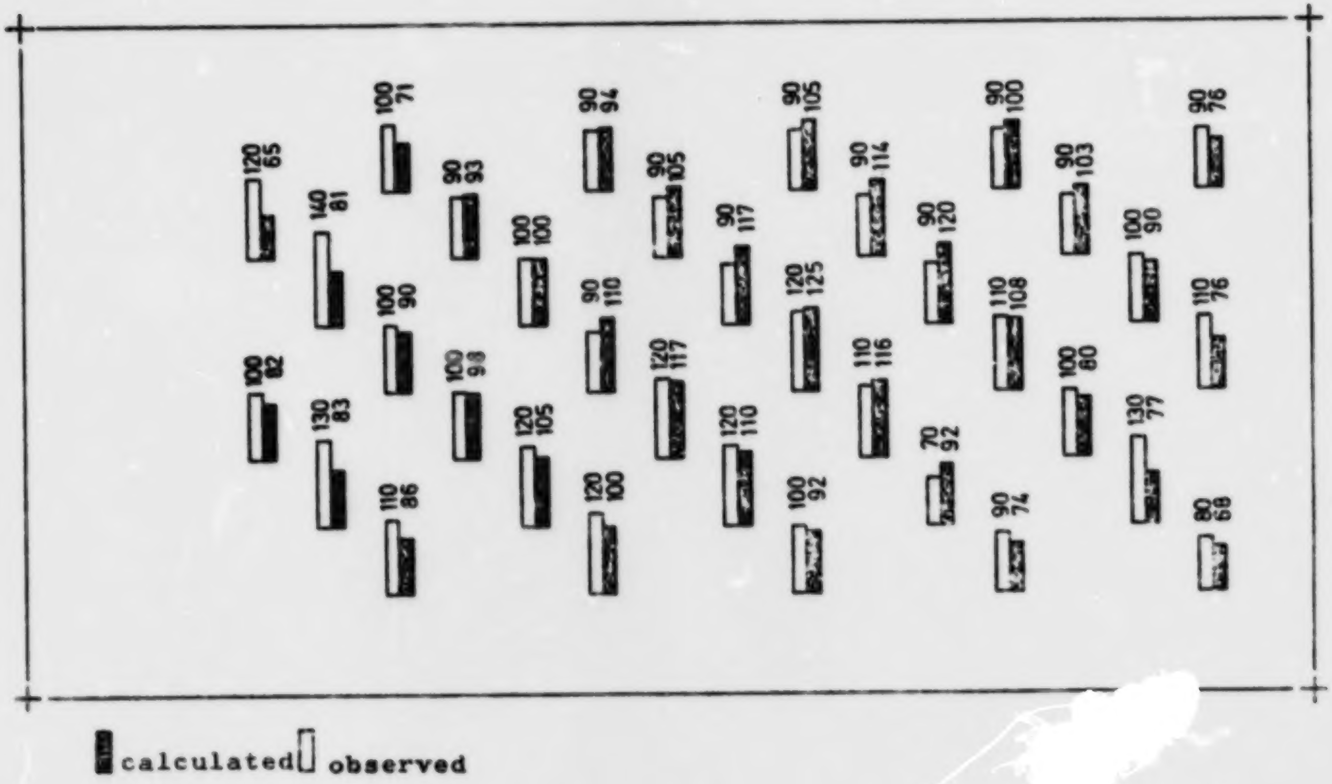

Fig. 4: Comparison of observed and calculated (AGDM, 1) annual mean concentrations ($\mu g/m^3$). Measurements made by Meß- und Prüfstelle, Kassel

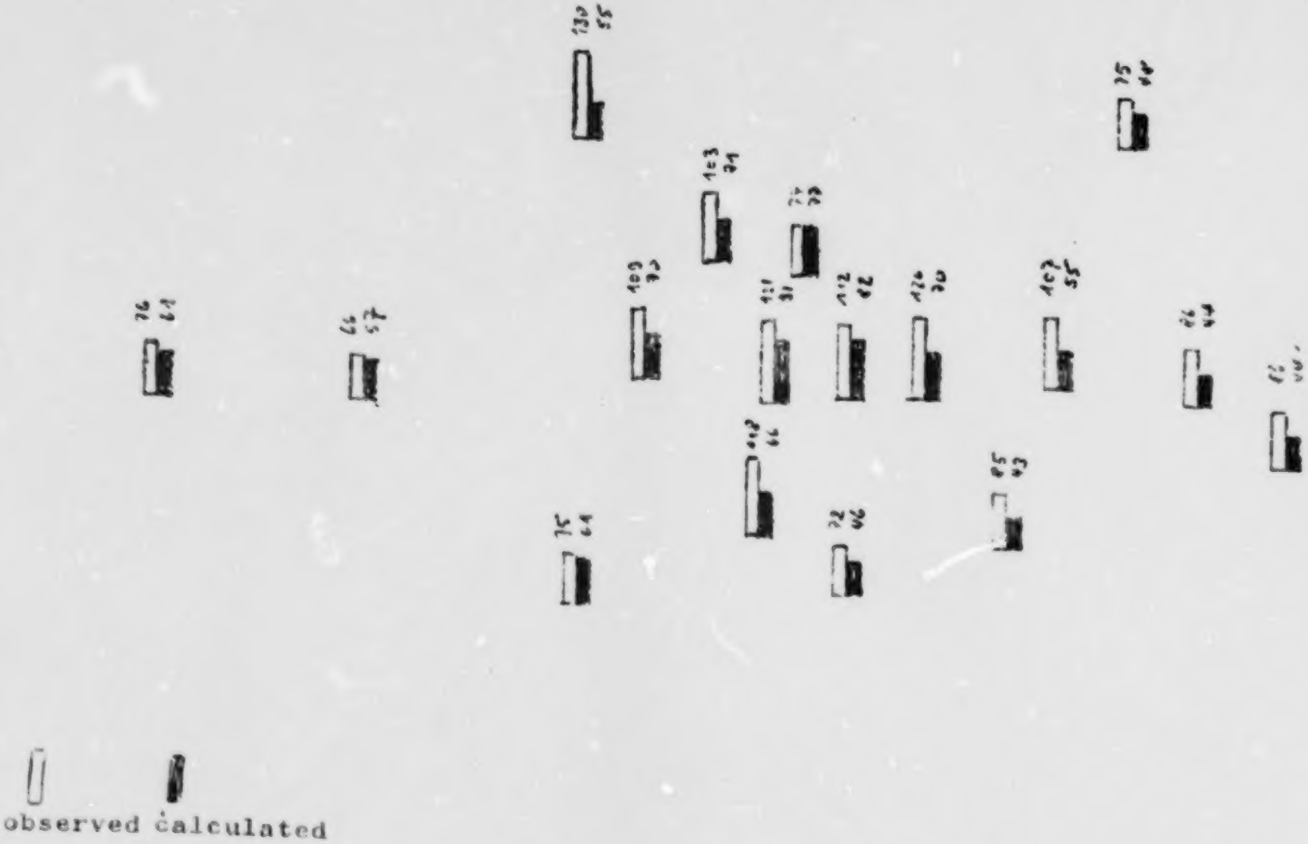

Fig. 5: Comparison of observed and calculated (AQDM, 2) annual mean concentrations (/ug/m³). Measurements made by Institut für Wasser-, Boden- und Lufthygiene, Berlin

Chapter 19

EPISODE PLANNING

by

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5th Meeting NATO/CCMS Expert Panel
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Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

EPISODE PLANNING

INTRODUCTION

Almost thirty years ago, Hewson described the role of meteorological factors that modify the behavior of air pollution once it enters the atmosphere. In the Trail investigation, he described the vertical stratification of sulfur dioxide in the early morning followed by dispersion shortly after sunrise. He also showed that wind, atmospheric stability, and topographic features influence the distribution of pollution.

Other well known examples of air pollution incidents, the Meuse Valley (1930); London (1952) (1956); Donora (1948); New York City (1953) (1963); to name a few, have demonstrated the importance of meteorological factors in the occurrence of undesirable levels of air contamination. Studies of these historical urban air pollution episodes have suggested that the simultaneous occurrence of very low wind speed, variable wind direction, pronounced stability and fog is characteristic of these episodes. Furthermore, these conditions persisted for several days and were associated with slow moving or stationary anticyclones (Niemeyer 1960). When the aforementioned meteorological conditions occur the dispersion of pollution released by various sources is generally limited, resulting in higher pollutant concentrations than occur normally.

METEOROLOGICAL ASPECTS OF AIR POLLUTION EPISODES

An air pollution episode may be said to occur whenever the atmosphere stagnates for a period of more than a day. The occurrence of atmospheric stagnation is often associated with a warm anticyclone. Warm anticyclones move slowly and have slow wind speeds through a deep layer. In general, warm anticyclones have little or no cloudiness associated with them and are without precipitation. The occurrence of subsidence (the slow sinking of air from the upper layers of the atmosphere) in a warm anticyclone also favors the occurrence of clear skies and the occurrence of ground-based radiation inversions. Together, these conditions produce a stable air mass with little horizontal or vertical mixing; and because of the slow meandering winds, pollution tends to remain near the emission source. The ambient concentration of quasi-stable pollutants depends upon the source emission rates, the height of the emission (near the surface or from a tall chimney), topography and the degree to which dispersion is limited.

In the United States, atmospheric stagnation tends to occur in preferred regions of the country and during certain months in a given region. In the eastern United States, the preferred region is the western slopes of the Appalachian Mountains where two to three cases of stagnation of four days or longer occur annually with ten to twelve stagnation days per year, mostly in the fall season (Korshover 1971). In the western United States, the preferred season for atmospheric stagnation is winter, except in the northwest where it is autumn. The meteorological potential for air pollution episodes is greater in the western United States than in other parts of the country and may average more than forty days per year. (Holzworth 1972).

Jost (1970) in a study of stagnating anticyclones over Central Europe reported the following frequency for a ten-year period: 35 times, lasting 3-5 days, 15 times lasting 5-7 days and 4 times lasting 7-10 days. The frequency is similar to the frequency found in the United States, particularly the eastern part.

It should be noted that the atmospheric stagnation occurs in many regions of the United States and Europe with a frequency of less than 5% of the days in a given year. However, as Meade (1959) noted, "With our present methods of fuel consumption, it needs only a suitable weather situation in winter for there to be a serious risk of smog. . . The notorious London smog of December 1952 lasted for only four days, but it was blamed for the deaths of 4000 people. The weather situation then was for the London area, unusual in its persistence, but no one can say it will not reoccur in 1, 5, or 10 years' time."

In the period since Meade made his statement, the world has made progress in the management of air quality. Outside events such as the discovery of natural gas in the North Sea and the gradual replacement of old inefficient factories and domestic heating methods have also had a marked influence on improved air quality. Nevertheless, it would appear to be imprudent not to consider the potential for a future air pollution episode and not to plan a course of action in the event one does occur.

EMERGENCY ACTION PLAN

In this section a "typical" Emergency Action Plan will be discussed. The intent is not to present a universal model plan, but to provide some insight as to what should be considered in designing and implementing a plan. Each city or political subdivision has special conditions which must be considered to meet local requirements. A more thorough discussion is available in three Environmental Protection Agency (1971) booklets entitled, "Guide for Control of Air Pollution Episodes."

The need for careful planning cannot be stressed enough. An air pollution episode is an unusual event and little time is available for reaction when the event occurs.

The precursor of an air pollution episode is the development of meteorological conditions leading to slow winds and atmospheric stagnation. Therefore, in the implementation of a plan to deal with extreme air pollution concentrations, primary consideration must be given to weather forecasts. The predicted duration of atmospheric stagnation is a major consideration as it can have an appreciable effect on the need for air pollution control actions. For example, during unfavorable situations in which the air quality is poor, whether or not remedial action would be taken, depends on whether or not the air quality would be expected to improve in a reasonable period of time by a change in the dispersive ability of the atmosphere.

In the United States large scale forecasts of atmospheric stagnation or high air pollution potential are provided by the National Weather Service on a daily basis. However, because of the detailed requirements of an emergency action, there is a need for local meteorological forecasts. The basic requirements for a real-time control strategy also include:

(a) Immediate availability of meteorological and air quality data

(b) A means of assessing the impact of various control strategies; e.g., a model

(c) Economic data assessing the effects of control activities

(d) Population distribution and potential health effects data

(e) A current emission inventory including the specific location of sources

(f) Control plans, including the lead time required for control actions to be applied by class, type and location of sources.

Emission inventories and specific plans for source reductions are vital for emergency control actions. The minimum control action taken should be sufficient to prevent damage to the health of the area's population.

In a typical city there will be a variety of sources emitting pollution. The only way to reduce pollution concentrations during an episode is to reduce emissions from the various sources in the area of concern. The control agency must, therefore, first determine the types and quantities of pollution being emitted, the lead time required to reduce emissions, and which sources can be controlled. The desired information must be obtained by the responsible agency through its emission inventory and requested from the major emission sources in the emission reduction plans they are required to provide.

Examples of emergency emission control actions which may be initiated during an episode are given below. Which of the actions should be implemented can be determined by a thorough review of the local control agency.

1. Prohibit open burning of trash, leaves, paper, or demolition debris.
2. Prohibit the use of Municipal, home, commercial, governmental, institutional, or industrial incinerators.
3. Delay start-up of new industrial equipment.
4. Postpone start-up and shut-down of industrial plants.
5. Lance bailers or blow soot only when it is absolutely necessary and then according to a schedule that takes advantage of the best meteorological dispersion conditions.

6. Reduce industrial processes that emit sulfur dioxide and/or fly ash to minimal operation.

7. Reduce consumption of all heating fuel, by decreasing indoor temperature to minimum comfort level.

8. Impose on the general population brown-out conditions comparable to those used during wartime.

9. Close down nonessential commercial, retail, and industrial establishments.

10. Prohibit the cleaning of storage vessels containing toxic or odorous compounds.

11. Enforce mandatory requirement that industrial batch operations discharging SO_2 be closed down.

12. Require bituminous coal users burning more than 2000 tons of coal annually to switch to low sulfur (1 percent or less) coal.

13. Require that all residual oil consumers who use more than 500,000 gallons of residual oil annually switch to low sulfur (1 percent or less) oil.

14. Require that natural gas be burned in those industries and power-generating facilities where gas and equipment are available.

15. Require that all power-generating facilities and all industrial units have a 5-day supply of low-sulfur (1 percent or less) fuels available for consumption of all times. This requirement would apply to any boiler or aggregate of boilers in one location whose total rated hourly capacity equals or exceeds, for example, 100,000 pounds of steam hourly.

16. Where possible, switch fuels in large stationary sources; e.g., power plants.

17. Import power from distant power plants outside of the episode area.

18. Limit the use of automobiles and other mobile sources.

EXAMPLE OF A TYPICAL EMERGENCY PLAN

Typical actions to be taken by a responsible control agency is presented in Figure 1.

The first indication of the potential episode is the forecast by the National Weather Service. The control agency prepares for a potential episode and advises major sources of episode possibility. The primary concern is to observe the trends in air quality levels.

If first alert air pollution levels are attained and meteorological information indicates that limited dispersion will continue for another 12 hours, the responsible control officer will call a first alert. Preventive actions are initiated. Public announcements are issued requesting the people to take precautionary measures and to limit their activities to curtail pollution emissions. Major sources are asked to switch fuels. Incineration and open burning is banned.

If the levels of pollution continue to climb, and if the weather forecast also indicates a continuation of the adverse conditions, a second alert stage is reached. At this stage health hazards begin to occur and more pronounced control measures are required. Industrial activities are requested to curtail or limit their operations. Mobile source limitations are implemented.

Hopefully, these preventive measures preclude the occurrence of the fourth stage and the necessity to issue a third alert. If a third alert stage were attained, it would be an emergency situation and would require the major curtailment of all non-essential activities in the community.

Once any status is reached, the control actions will remain in force until adequate ventilation has been restored and air quality levels are again within acceptable limits.

CONCLUDING REMARKS

Several points should be emphasized:

1. Air pollution episodes are still a real problem and may be expected to occur again when the appropriate source and weather conditions occur simultaneously.
2. Meteorological surveillance is an available technique which should be used.
3. The reaction time for an agency to act is small; but with a plan of action, the severity of an air pollution episode can be significantly reduced.

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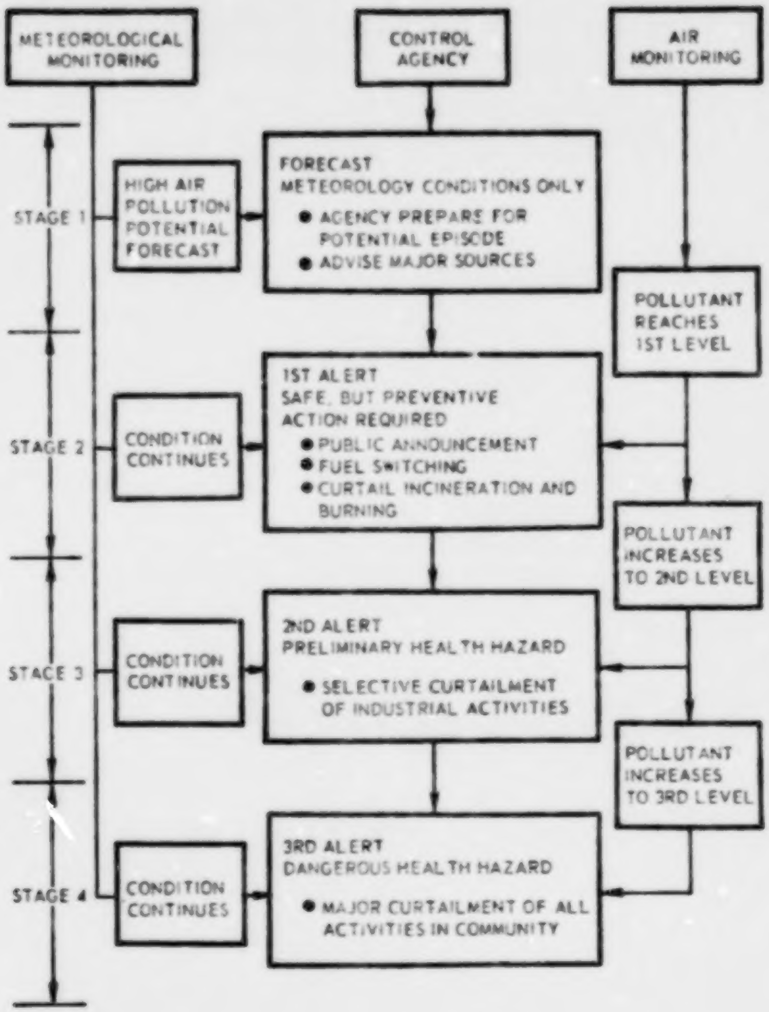
METEOROLOGICAL MONITORING
CONTROL AGENCY
AIR MONITORING
STAGE 1
HIGH AIR POLLUTION POTENTIAL FORECAST
FORECAST
METEOROLOGY CONDITIONS ONLY
● AGENCY PREPARES FOR POTENTIAL EPISODE
● ADVISE MAJOR SOURCES
POLLUTANT REACHES 1ST LEVEL
STAGE 2
CONDITION CONTINUES
1ST ALERT
SAFE, BUT PREVENTIVE ACTION REQUIRED
● PUBLIC ANNOUNCEMENT
● FUEL SWITCHING
● CURTAIL INCINERATION AND BURNING
POLLUTANT INCREASES TO 2ND LEVEL
STAGE 3
CONDITION CONTINUES
2ND ALERT
PRELIMINARY HEALTH HAZARD
● SELECTIVE CURTAILMENT OF INDUSTRIAL ACTIVITIES
POLLUTANT INCREASES TO 3RD LEVEL
STAGE 4
CONDITION CONTINUES
3RD ALERT
DANGEROUS HEALTH HAZARD
● MAJOR CURTAILMENT OF ALL ACTIVITIES IN COMMUNITY

Figure 1. Four Stage Alert Sequence

Chapter 20

AN INTRODUCTION TO THE VENICE AIR POLLUTION PROJECT

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

AN INTRODUCTION TO
VENICE AIR POLLUTION PROJECT

E. Runca- IBM Scientific Center
Venice - Italy

1) Introduction

Many attempts have been made during last few years in order to relate the air quality of an industrialized and urban region to the emissions and to the local meteorological conditions. This led up to the development of multisources diffusion models. Some common items can be identified though the Air Quality Diffusion Models differ in theoretical approach or in the kind of smog to be described.

Every AQDM is based upon an available Data Bank that must provide an input to the simulation of the phenomena and to the validation of the model output. The AQDM structure is shown in fig. 1.

The implementation of an AQDM has mainly the objectives of:
- providing a tool used by policy planners to take decision;
- providing a tool to be used in an alert system.

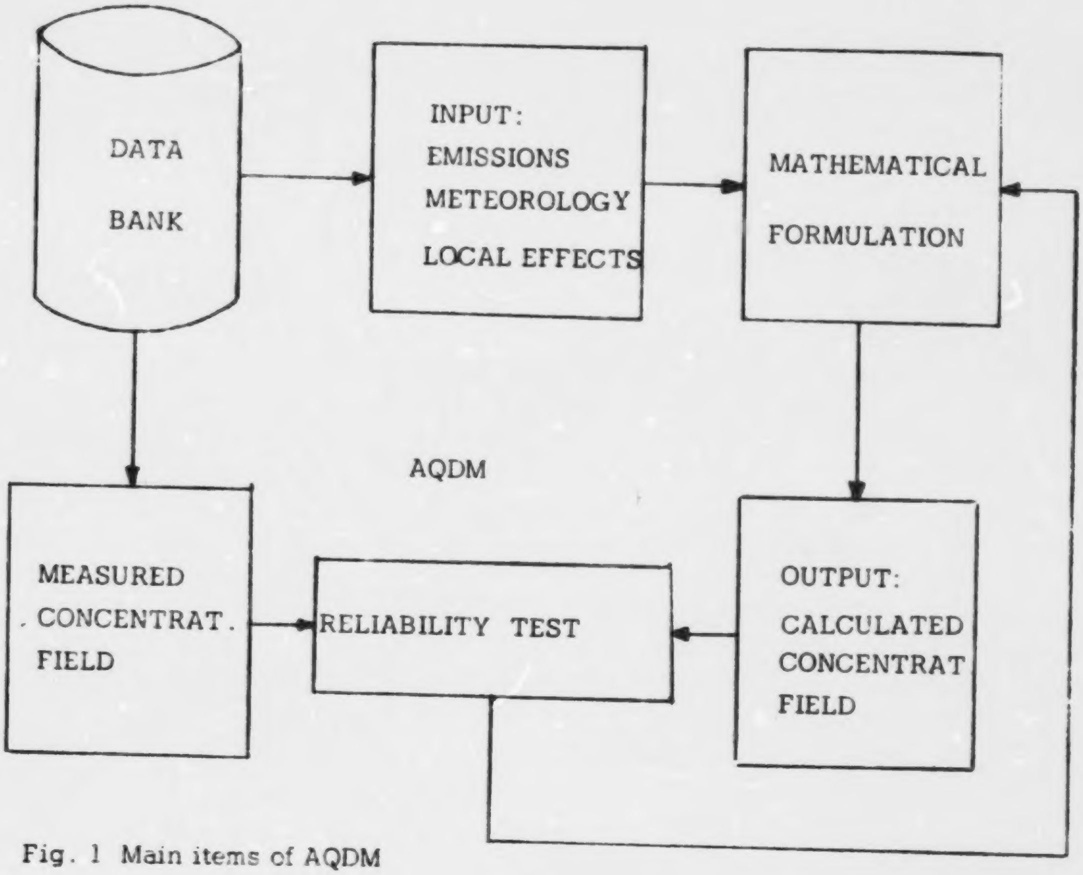

DATA
BANK
INPUT:
EMISSIONS
METEOROLOGY
LOCAL EFFECTS
MATHEMATICAL
FORMULATION
AQDM
MEASURED
CONCENTRAT.
FIELD
RELIABILITY TEST
OUTPUT:
CALCULATED
CONCENTRAT
FIELD

Fig. 1 Main items of AQDM

In order to achieve the objectives above listed the AQDM must be implemented together with other tools and models, such as, for instance, an abatement strategy model and a mesoscale meteorology predictive model, so that, an Air Quality Management System, can be obtained. Nevertheless the AQDM simulating the concentration field is a powerful tool which can be used without collateral models as a help for decision makers or in an alert system. Thus the reliability of an AQDM should be emphasized.

Because of the lack of a well-established turbulent transfer-theory in the lower atmosphere the reliability of the model can be tested only by confrontation between the calculated concentrations and the measured ones. Therefore the relevance of a consistent data bank both for validating new models and for the management of environmental problems is quite apparent.

As a consequence of the above conclusions the IBM air pollution project for Venice, whose main objective is the design of an AQDM, has been extended to the organization of a compatible and easily accessible Data Bank. The following is a summary of what has been done up to now in order to understand and to describe the Venice Air Pollution Problem.

2) The Venetian area

The area under investigation, shown in fig. 2, is located in the Veneta Lagoon between the Veneta plain and the Adriatic Sea and is quite flat. The only geographical discontinuities are due to the presence of the urban and industrial complexes in the area. The urban areas are formed by Venice, Mestre and Marghera. The industrial facilities are adjacent to the urban areas of Mestre and Marghera and are separated from Venice by a Lagoon strip about 5 Km. wide.

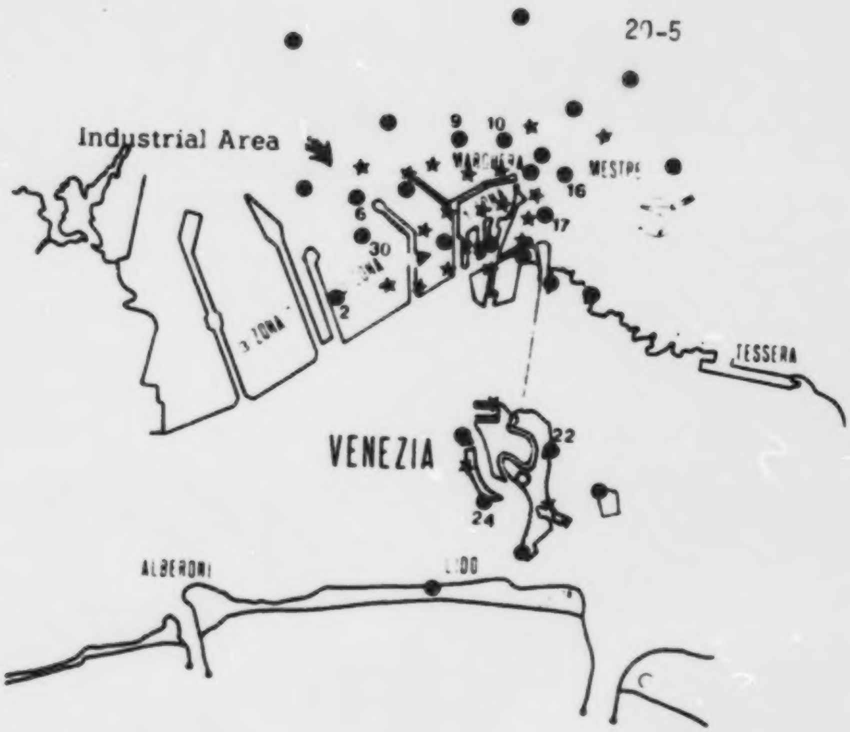
3) The Air Pollution Problem of Venice

The interest in investigating the dispersion patterns of the gaseous effluents released into the Venetian atmosphere arises from the damages that a polluted atmosphere can exert on the priceless Venice artistic patrimony, as well as from reasons of public health.

The pollutants originate from residential and industrial activities. The inhabitants of the Venetian area are about 400,000, one third of whom are living in the historical center. The emissions of residential origin are due to domestic heating and automotive sources (the latter in Venice are motor-boats).

The firms, mainly located in the industrial zone, are about 230 and employ appoximately 50,000 workers.

Their activities belong to the following fields:
- chemical products;
- oil refineries;
- food stuffs;
- metallurgy of iron and other metals;
- coke and glass industry;
- power plants.



● ISS-Tecneco SO_2 sensors

○ ISS-Tecneco meteor. station

★ Ind. Committee: SO_2 sensors

✱ Ind. Committee: meteor. stations

▲ Ind. Committee: meteor. tower

FIG. 2

Up to now a comprehensive survey of the pollutants discharged inside the Venetian atmosphere is not yet available. Disregarding at the moment the kind of pollution afflicting Venice, the objective of a diffusion model designed for the area must be the understanding of the residential and industrial relative contributes to the pollution level and of the way in which any change in the residential and industrial activities affects it.

Hence the AQDM should provide a guideline for the future development of the facilities located in the industrial zone. Along with the previous problem there is the need of defining a pollution level not dangerous for artistic patrimony.

Up to now the only pollutant whose concentration has been extensively recorded is sulphur-dioxide, since, according to preliminary results, it seems that the decay of stone in Venice is due to its reaction with SO_2 yielding sulphates.

In addition to that, SO_2, because of its poor reactivity can be considered a tracer of the dispersion patterns, which explains the installation of so many SO_2 - detecting stations.

4) Monitoring networks in the Venetian area

At present there are two main monitoring networks controlling air quality. One of them has been installed by Tecneco, a private company, under the commission of ISS (Istituto Superiore Sanità); the other one has been installed by Ente Zona Industriale Porto Marghera (Planning Committee of the Industrial Area).

The ISS-Tecneco (+) begun to operate in 1973 and at present has:

- 24 SO_2 sensors
- 2 NO_x sensors
- 1 meteorological station

over an area of about 300 Km^2 (see fig. 2); ten of the twenty-four SO_2-sensors aad the meteorological station begun to transmit in February '73, the remainder in March '74. The sensors are scanned by a small computer that stores the hourly average values and the worst 30-minutes SO_2 concentration. The SO_2 data are weekly published on the local newspaper.

The network installed by the industries (see fig. 2) begun to operate in April '74 and consist of:

- 21 SO_2 sensors;
- 1 NO_x sensor
- 4 meteorological stations;
- one meteorological tower where up to now only temperature is measured at 10,70 and 140 m.

The data are transmitted to a small computer in a way similar to the previous network.

Besides the two main networks there are two meteorological stations of the Italian Meteorological service, one of which is located at Tessera airport in the mainland, the other one located at S. Niccolò airport in Lido.

There are also some private meteorological stations from which it is possible to gather information.

5) Preliminary results

Meteorology

An analisis of a set of meteorological data registered at the two stations of the Italian Meteorological Service and at a private station located at Lido has been carried out in order to get some preliminary information about the local climate.
For each station ten years data have been stored on a magnetic tape and have been analyzed. The results are similar for the three stations and they are briefly illustrated by figures drawn with the data registered at Tessera airport station (figs. 3,4, 5).

(+) ISS-Tecneco is also carrying out an analysis of the rain fall and is collecting data on suspended particles.

TESSERA

PERIOD 61-71 TRI-HOURLY DATA

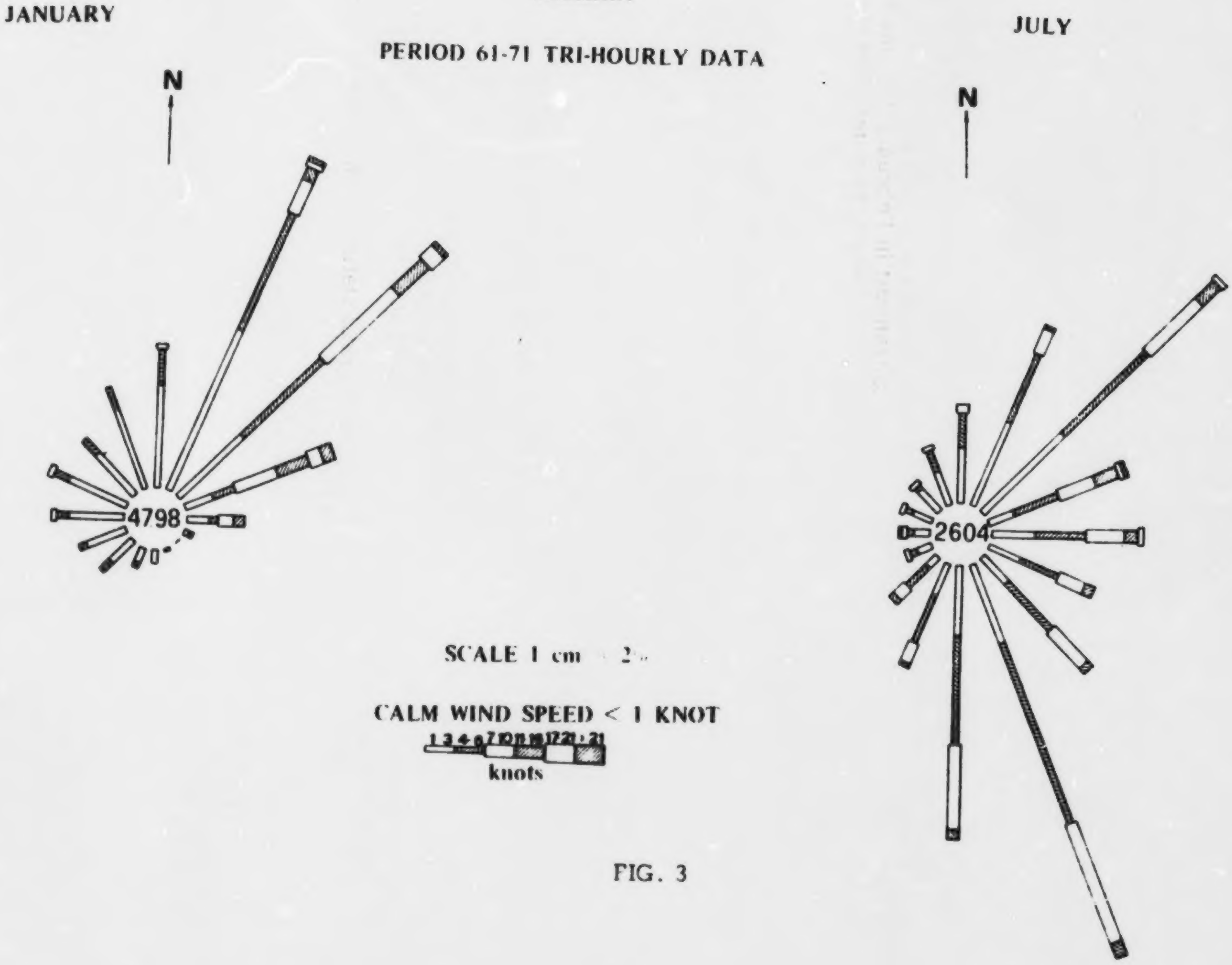
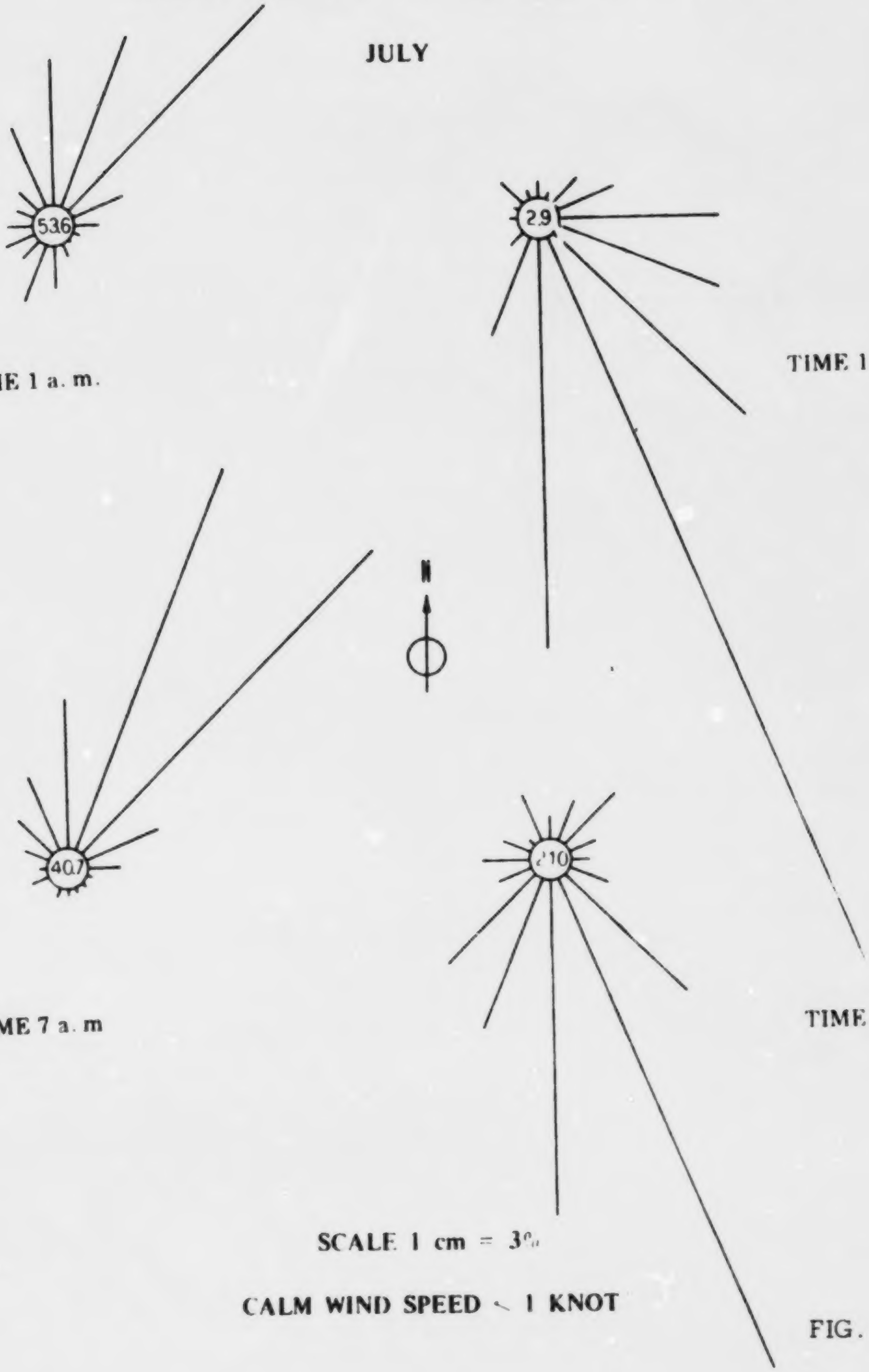


FIG. 3

TESSERA PERIOD 61-71 TRI-HOURLY DATA

JULY



TIME 1 a. m.

TIME 1 p. m.

TIME 7 a. m

TIME 7 p. m.

SCALE 1 cm = 3%

CALM WIND SPEED < 1 KNOT

FIG. 4

The monthly and yearly distribution of wind direction, wind speed, temperature, pressure, relative humidity, visibility, atmospheric stability were computed. The results show a seasonal pattern. The analysis indicated that during winter months there is an accentuation of those factors generally recognized as essential for the accumulation and stagnation of the pollutants released into the athmosphere, i.e.: low wind speed, stable conditions, high pressure system.

The wind roses drawn for every month show that during the no-heating seasons the wind from the Adriatic Sea to Venice is rarely blowing while it is blowing most of the time during the heating-seasons (see fig. 3).
Hence a sea breeze effect is characteristic of the area and this has been made apparent in fig. 4, where the wind roses corresponding to the local hours 01-07-13-19 have been calculated for July. For the latter ones only winds having speed lower than 10 Km/h have been taken into account.
The clockwise rotation of the wind direction during the day is due to a sea breeze effect. A main feature of the area is the high percentage of calm conditions and light winds (see fig. 5). The main conclusion of the performed analysis is that the design of an Air Quality Diffusion model for Venice should be able to handle very low wind speed situations and the dynamic of a sea breeze effect.

TESSERA PERIOD 61-71

TRI-HOURLY DATA

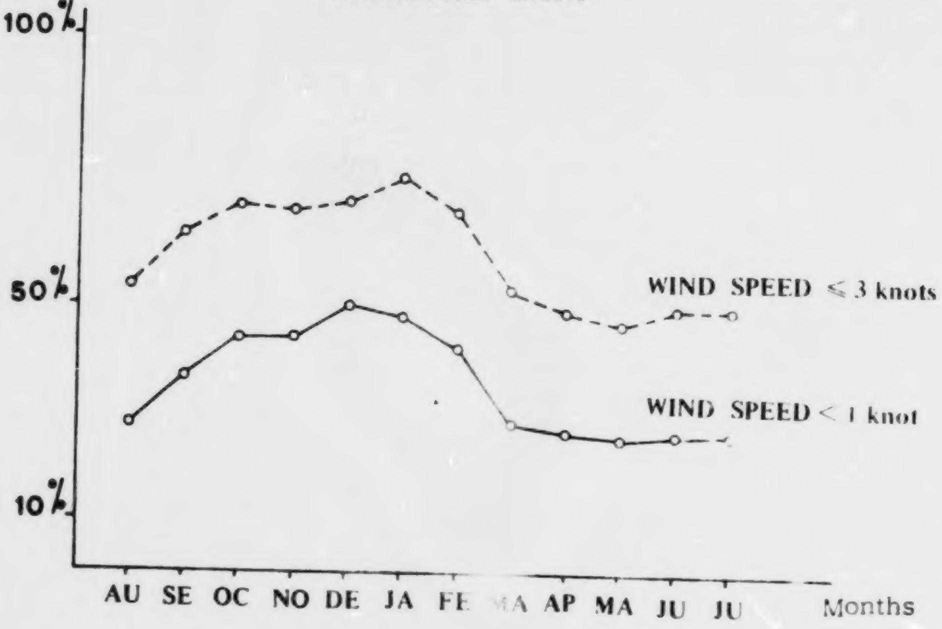


FIG. 5

- Pollution

As above pointed out the only pollutant widely recorded is sulphur dioxide. Before the installation of the two main networks SO_2 data had been already collected by private factories and local institutes. They mainly consisted of 24 hours average values showing that it is possible to reach in the area high SO_2 concentrations. The SO_2 concentration data made available by ISS-Tecneco confirm that 30-minutes average values close to 1 ppm can be measured. Table 1 shows how many times the maximum 30-minutes and daily average values estabished by the Italian law, (0,30 and 0,15 ppm respectively) have been overcome at ten ISS-Tecneco stations during the period February '73- January '74.

- Emissions inventory

According to the Italian law for the regulation of atmospheric pollution the factories must supply the local authority with data concerning the geographical disposition, the geometry and the emission composition of their sources.

At present the local authority of the "Regione Veneta" is drawing up an inventory of the industrial emissions with the consulence of the IBM Scientific Center, Venezia. A form designed according to the Italian law has been already sent to every firm and the inventory should be completed within the present year (+). Some already available data from 75 industrial sources give the figure of about 150,000 tons/year of SO_2. Any reliable data concerning the emissions originating from residential activities are not up to now available. The data about residential activities seem to be quite uninteresting since, according to the above mentioned Italian law, methane or natural gas must be the only energy source for domestic heating in Venice.

Some unofficial information suggests that the amount of SO_2 due to residential activities is about the 5% of the total SO_2.

6) Modeling efforts

At present a very simple air quality diffusion model has been designed with the purpose of testing the applicability of some already experimented techniques in this area. The model uses as an input the meteorological data recorded at ISS-Tecneco station and the rough SO_2 data of the 75 industrial emission mentioned in the previous paragraph. The output of the model consists of the daily SO_2 concentrations at the locations of ISS-Tecneco SO_2 monitoring stations.

(+) The inventory will provide the emitted amounts of SO_2, CO, NO_x, hydrocarbons and other pollutants.

Sensor	Feb.73	Mar.73	Apr.73	May 73	Jun.73	Jul.73	Aug.73	Sep.73	Oct.73	Nov.73	Dec.73	Jan.74
SO_2 - Daily average concentrations greather than 0.15 p p m												
2	2	0	0	0	0	0	0	0	2	1	4	1
6	3	0	1	0	0	0	0	0	2	0	1	2
9	0	8	2	2	1	0	0	0	0	0	0	1
10	3	4	1	0	0	0	0	0	0	0	4	1
16	0	0	1	0	0	0	0	0	0	0	3	7
17	0	0	0	0	0	0	0	0	0	0	0	2
22	0	0	0	0	0	0	0	0	0	1	0	3
24	0	0	0	0	0	0	0	0	0	0	0	0
29	0	1	1	0	0	0	1	0	2	4	8	2
30	4	2	1	0	0	0	0	0	0	0	0	6
SO_2 - 30 minutes average concentrations greather than 0.30 p p m												
2	15	9	3	2	1	6	5	8	12	13	32	12
6	11	22	12	2	2	9	9	2	20	0	10	4
9	7	81	49	66	18	13	22	12	0	4	0	9
10	17	34	22	34	3	6	10	13	2	4	6	10
16	9	9	19	2	1	0	1	3	1	18	4	22
17	3	2	21	3	0	2	2	8	2	5	0	17
22	1	1	3	0	0	2	0	1	2	19	5	27
24	0	1	0	0	0	0	0	0	0	4	4	2
29	11	31	31	17	2	12	16	7	40	63	48	10
30	20	22	34	8	18	35	12	11	21	3	0	1

TABLE 1

The matematical formulation assumes that the pollutant has a gaussian distribution in the vertical and is unformly distributed crosswind. The latter assumption implies that the wind direction has uniform distribution in each sector of the wind-rose. With the above assumptions the working equation of the model has been written as follows:

$$C(R)=\sum_{P=1}^{M}\left[\frac{Q(P)\cdot N}{2^{1/2}\,\pi^{3/2}\,u\,S_z\,D_{P,R}}\exp\left(-\frac{H^2(P)}{2\cdot S_z^2}\right)\right]$$

where:

M	number of point sources
$C(R)$	hourly average concentration ar receptor point R
$Q(P)$	emission rate of the source P
N	number of wind rose sectors (N = 8, in the ISS-Tecneco station)
S_z	vertical standard deviation
u	wind velocity
$D_{P,R}$	projection along the wind direction of the distance between the receptor point and the point source
$H(P)$	effective height of the source P

Eq. (1) is used to compute 24 values of concentration at the receptor point R. The arithmetic mean is then assumed as an estimate of the daily average value. In the model the stability classes are defined according Pasquill and S_z is expressed by an exponential law. Up to now the model has been run only a few times and needs some improvements. Some results are shown in fig. 6 , but our experience with this model is still too little to enable us to draw any conclusion on its reliability.

7) Future work

- Data Bank

As above described the amount of data collected in this area is quite considerable and it is evident that in order not to waste them they must be stored in a data bank. The relevant role of a data bank in an air quality management system has been discussed briefly in the introduction.

The usefulness of a data bank is strongly dependent upon the organization of the information collected in it and the available software to update and inquire it. The users of this kind of data bank are scientists and policy planners. Because the latter ones are the most important users, the implementation of the data bank must mainly take into account their needs. Thus the approach we are following intends to free the users from the constraint of being aware of the data structure, or in other words the data should be completely transparent to the user. Preliminary discussion about this project suggest that an approach based on relational concepts should meet our requirements.

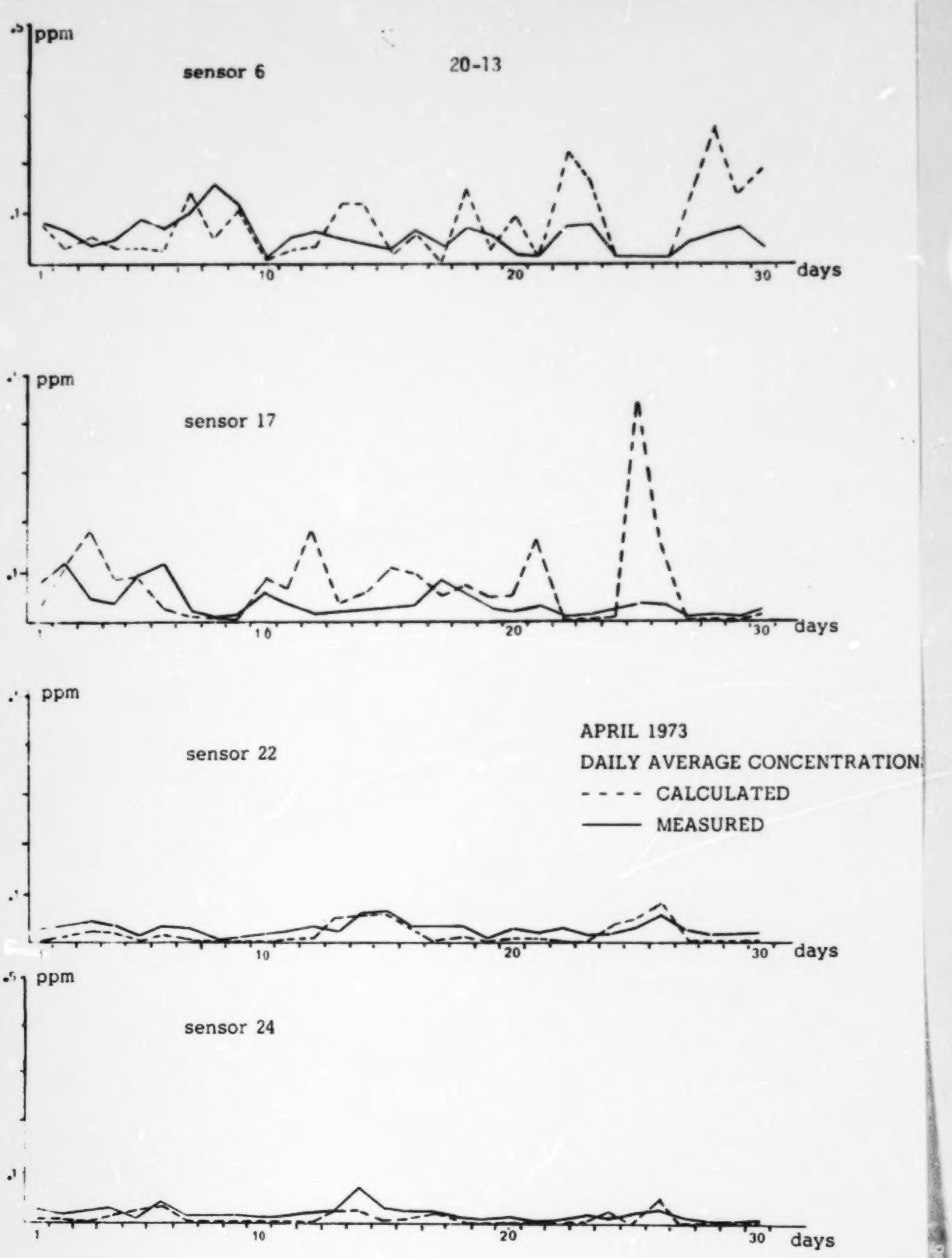

20-13
.5 ppm
sensor 6
.1
1
10
20
30
days
ppm
sensor 17
.1
1
10
20
30
days
ppm
sensor 22
APRIL 1973
DAILY AVERAGE CONCENTRATION
- - - - CALCULATED
—— MEASURED
1
10
20
30
days
.5 ppm
sensor 24
.1
1
10
20
30
days

FIG. 6

- **Modeling techniques.**

Along with the validation of the simple Gaussian kind diffusion model an effort will be done to implement an air quality model able to incorporate the main features of the local air dynamics. The design of such a model requires more accurate data than the ones collected up to now. It seems that the emissions inventory organized by the local authority; the data gathered by the two main networks and some other measurements planned by the CNR (Consiglio Nazionale Ricerche) will supply the required data. We are strongly convinced that an effort should be made to understand the influence, mainly during calm conditions, of the heat-islands effects caused by Mestre-Marghera-Industrial zone and Venice and the breeze effects upon the dispersion of pollutants in the area examined.

Acknowledgements

Sincerest appreciation is expressed to Tecneco S.p.A. which supplied the above reported experimental results and to Dr. Zannetti of IBM Italia for his general contribution to the project.

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Chapter 21

URBAN PLANNING UTILIZING A REGIONAL ATMOSPHERIC SIMULATION MODEL

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
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URBAN PLANNING
UTILIZING
A REGIONAL ATMOSPHERIC SIMULATION MODEL

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Delivered by A.E. Boyer at the Eighth Annual Congress, Canadian Meteorological Society held at York University, May 29 - 31, 1974

URBAN PLANNING UTILIZING A REGIONAL ATMOSPHERIC SIMULATION MODEL

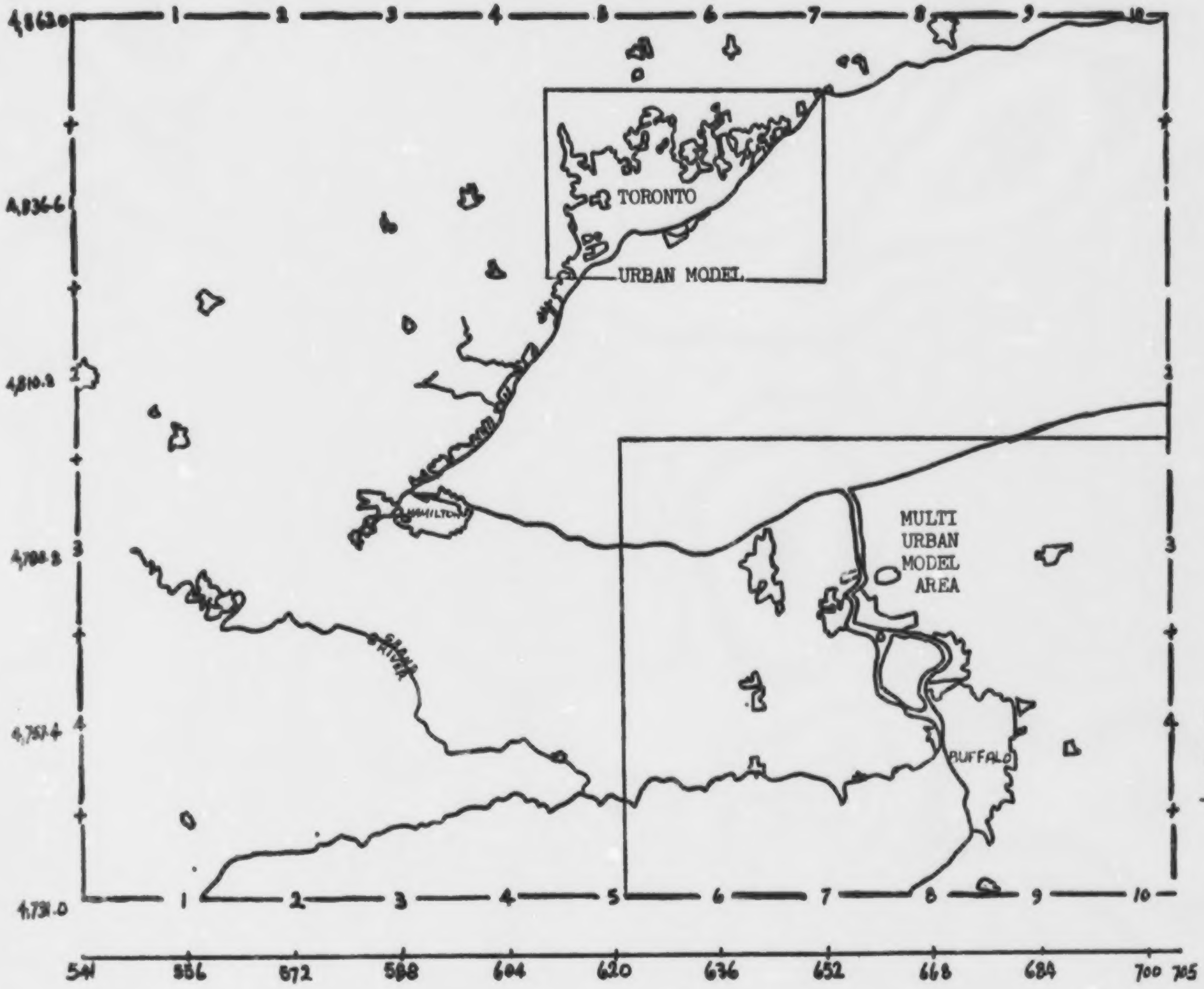
Introduction

Since 1969, the Air Resources Branch of the Ontario Ministry of the Environment has developed and utilized a series of Urban Air Quality Simulation Models (1, 2). More recently these models have been expanded to cover multi-urban and regional simulations. This has been made possible by the completion of a pollutant inventory for the area from Toronto to Hamilton and the Niagara Peninsula of Ontario as well as an interface with the pollutant inventory for the State of New York. The dimensions of these models, shown in Map 1, range from 40 kilometers for the urban model to 160 kilometers for the regional model, the multi-urban model falling mid-way between the two.

As the scale of simulation models increase the relative importance of several factors change:

1. Mixing depths, relatively unimportant in a properly designed urban area, become increasingly important in evaluating the growth of an urban plume.
2. Tall stacks, of great use in controlling urban air quality, are much less effective in altering the air quality on regional scales of 50 to 200 km.
3. Land use planning, of limited effectiveness in controlling the transport of pollutants on an urban scale, is of vastly increased importance in regional urban planning.

Grid increments of one, two, and four kilometers have been chosen for the urban, multi-urban, and regional models respectively. At distances of less than two grid units from very large sources, this grid


4,862.0
4,836.6
4,810.8
4,783.8
4,757.4
4,731.0
541
556
572
588
604
620
636
652
668
684
700
705
1
2
3
4
5
6
7
8
9
10
TORONTO
URBAN MODEL
HAMILTON
GRAND RIVER
MULTI URBAN MODEL AREA
BUFFALO

Map 1
Area Covered by
Ontario Regional
Simulation Model

164 X 132 Km

square averaging tends to smooth out maximum concentrations thus making it imperative to avoid the study of strictly urban problems with a regional simulation model.

When considering the impact of a large source on the urban environment, the maximum ground level concentration produced by that source, or the impingement concentration on some nearby structure are limiting considerations. When considering the downwind impact of an urban plume on another urban area, we are far removed from the maximum GLC and are instead confronted with the cumulative effects of numerous overlapping plumes. In this region, the effect of a remote tall stack may be insignificant, while the effect of the vertical temperature structure of the atmosphere in determining the growth of an urban plume assumes a new importance, and, finally and perhaps most important, the impact of the geographical distribution of land use on the cumulative effect of overlapping sources can be pronounced if a series of large sources are aligned parallel to regional wind trajectories.

Downwind Impact of an Urban Plume

Munn (3, 4) and others (5) have discussed the existence of an "urban plume" downwind of urban centers. It has been suggested that complete evaluation of the impact on air quality of an urban center must consider effects over distances as great as 200 km. If this is true, evaluation of pollution control strategies and land use planning requires consideration of scales greater than the 40 km which encompass present urban air quality models. The evidence for this conclusion is not overwhelming. An investigation of the impact of SO_2 sources located in Toronto on receptors in Hamilton, 60 km distant, tends to confirm the conclusion of Munn, but only for certain circumstances.

Walli has reported (6) the impact of various sources along the Toronto - Hamilton axis on receptor points in Hamilton. For a northeast wind, parallel to the Toronto - Hamilton axis, simulated concentrations of SO_2 at some receptor points in Hamilton were as high as 24 pphm, with sources such as a Toronto power station, 46 km distant, contributing more than 10 pphm. (See Table 1, "Major Contributors of SO_2 Concentrations - Receptor Point UTM 91 - 89).

At this same receptor point, space heating emissions from local commercial land use, were responsible for 3 pphm; a refinery, 17 km northeast of Hamilton added 3 pphm. Two industrial complexes and another refinery at distances between 17 and 38 km each, contributed about 1 pphm; 2,000 other sources combined to add another 3 pphm to the total of 24 pphm. These simulated concentrations of SO_2 do lend credence to the idea that urban areas at distances comparable to that between Toronto and Hamilton, do affect the air quality of the next urban area downwind.

These results can be explained in part by the fact that the Toronto - Hamilton wind trajectory chosen for investigation, is also parallel to the Lakeshore along which commercial and industrial development has concentrated as shown in Map II "Location of Major SO_2 Sources". Obviously, for other wind trajectories, Toronto sources would not have affected Hamilton and, in fact, no alignment of sources, except along a NE - SW line would produce such an accumulation of overlapping of source plumes. Unfortunately winds from the SW or NE occur more than 30% of the year. Changnon (7), in his study of the LaPorte weather anomaly, states that during the warm season, Lake Michigan produces a dome of cold air which, coupled with westerly and southwesterly flow, creates a convergence zone parallel to and just inland of the lake shore. Thus, any tendency for wind trajectories

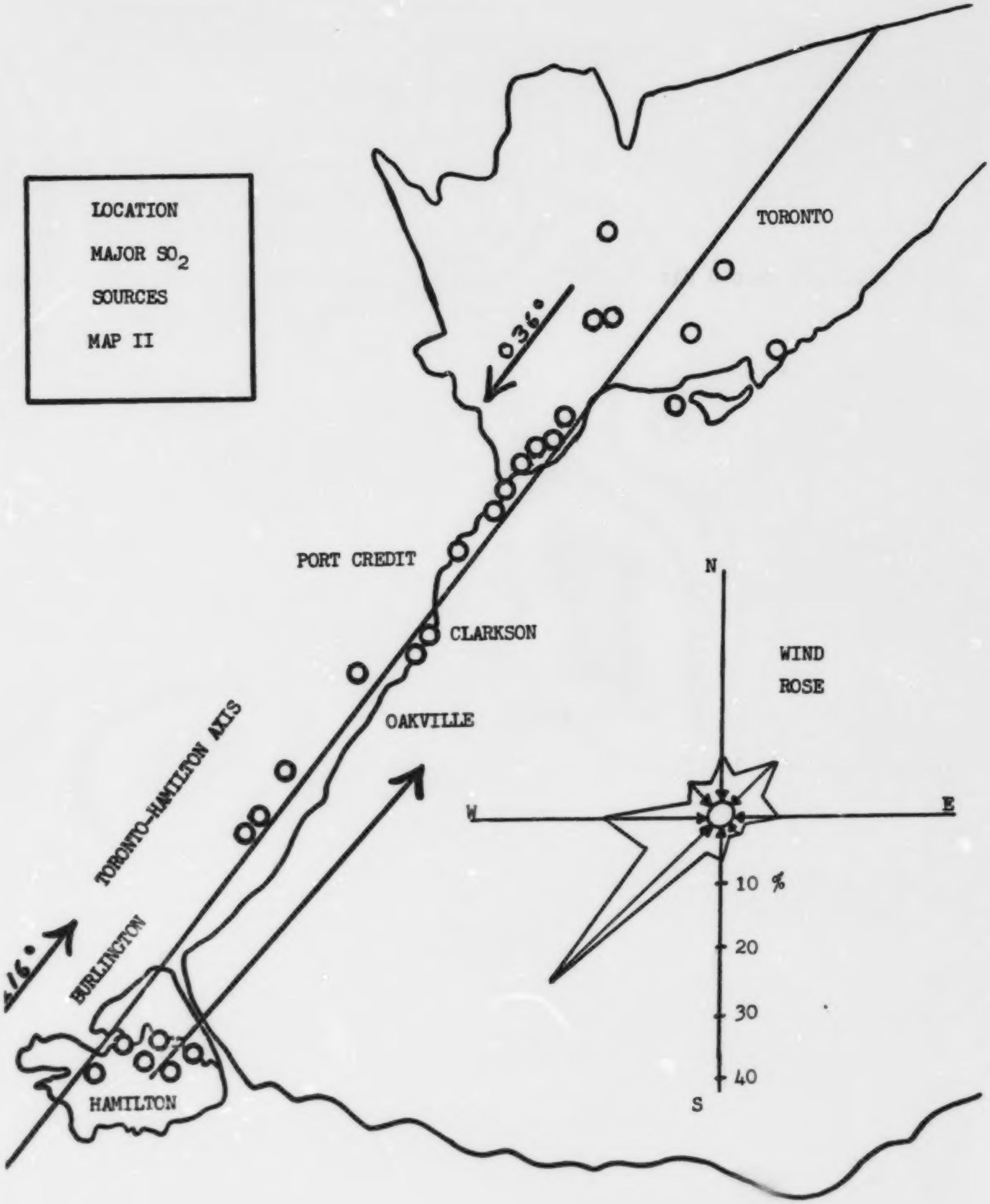
TABLE 1

Major Contributors to SO_2 Concentrations

Receptor Point UTM 91-89

Wind 036°/14 mph (selected to maximize non local sources)

SOURCE	LOCATION	CONTRIBUTION PPHM SO_2	SOURCE DISTANCE km.
Power Station	Toronto	11.4	46
Land use - Commercial Buildings	Hamilton	2.8	1
Refinery	Burlington-Oakville	2.8	17
Industrial Complex	Clarkson	1.6	32
Refinery	Burlington-Oakville	1.1	17
Industrial Complex	Port Credit	0.6	38
Public Building	Hamilton	0.3	1
Industrial Firm	Hamilton	0.3	1
Land use - Commercial Buildings	Hamilton	0.2	2
2000 Other Sources	Toronto to Hamilton	2.7	
		23.8 pphm	



LOCATION
MAJOR SO_2
SOURCES
MAP II

TORONTO
036°
PORT CREDIT
CLARKSON
OAKVILLE
TORONTO-HAMILTON AXIS
216°
BURLINGTON
HAMILTON
WIND
ROSE
N
W
E
S
10 %
20
30
40

to parallel the lakeshore from Toronto to Hamilton, will magnify the cumulative effects simulated above.

The type of meteorological conditions which tend to conserve an urban plume for long distances, and those wind trajectories which are conducive to the overlapping of many large sources, are subjects which meteorologists should direct their attention to in the coming decade. The variables which appear to be important are the mixing depth, the horizontal wind trajectories, and the vertical velocity profile. In short, what is required is a more sophisticated three-dimensional meteorological model.

Mixing Depth Effects - Urban and Regional Differences

As soon as pollution control engineers and meteorologists recognized that the combination of shallow mixing depths and low elevation sources produced episodic levels of air pollution, taller stacks, higher exit temperatures, and all changes to produce higher effective stack heights were used to avoid the recurrence of such events. These programs were so effective over the past decade, that the limiting case of a low level inversion and a calm atmosphere, although still much talked about, no longer produces the highest levels of pollution in urban areas. In many cities, such as Windsor, Sudbury, and Welland in Ontario, highest pollution levels occur with unlimited mixing depths and moderate to strong winds. There are still some cases in which low elevation mixing depths and light winds produce highest concentrations. Noteable among these are low elevation discharges from foundries and smelters, coke ovens, and small heating plants (especially those burning coal).

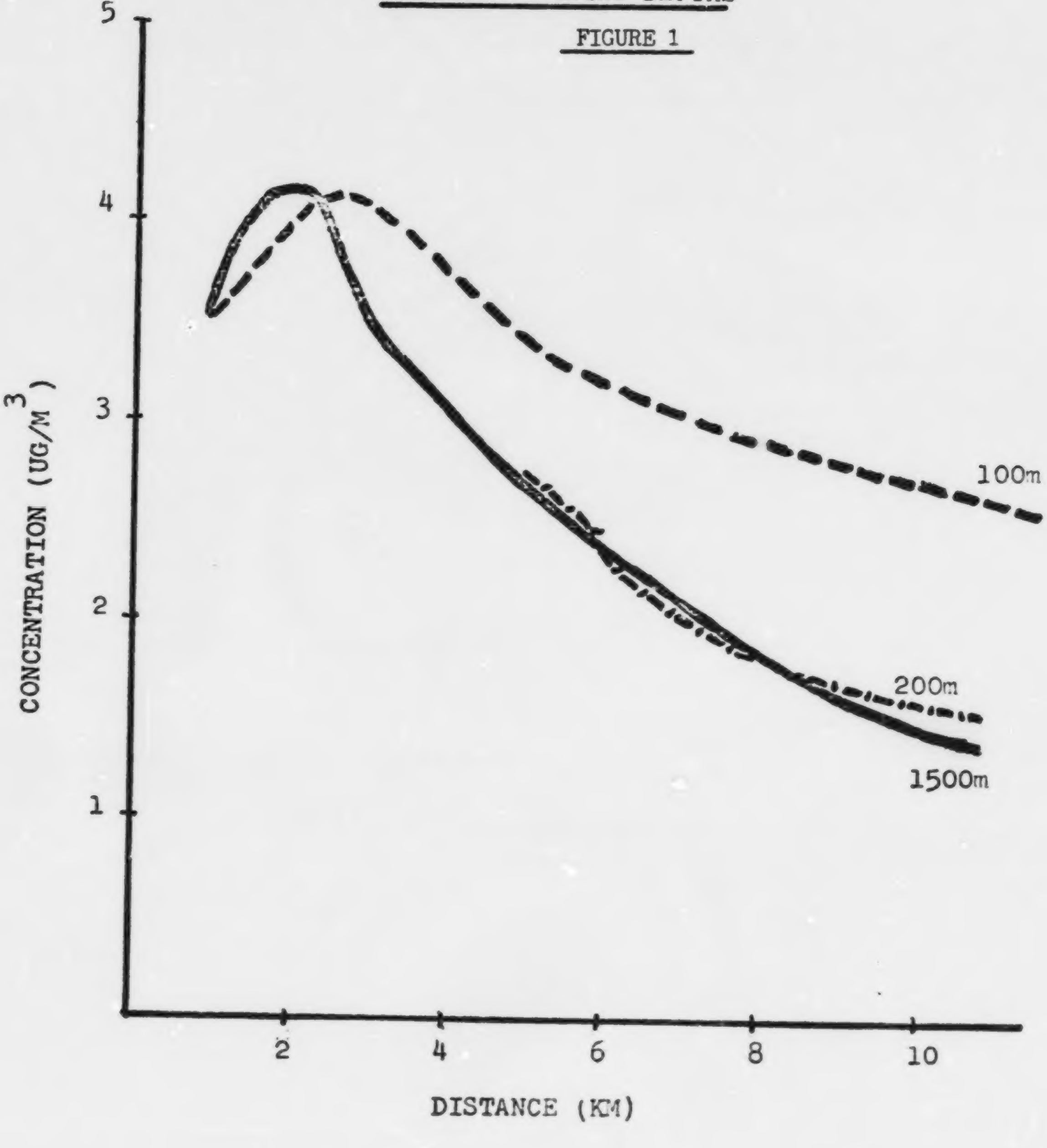
Using the Hamilton Atmospheric Simulation Model as a diagnostic tool, a simulation of various combinations of mixing depth, stack height, and wind speed showed that for a 100 m stack, the mixing depth variance between 200 and 1500 m had no significant effect on the maximum downwind concentration occurring at a distance of about 5 km.

For smaller stacks of 30 meters, there was still no significant effect on the maximum downwind concentration but at a distance of 10 km there was a noticeable increase in concentrations for those tests in which the mixing depth was as low as 100 meters. This is shown in fig. 1, "Downwind Concentrations for Three Mixing Depths". From the standpoint of urban simulations, the fact that lowering the mixing depth to 100 meters doubles the concentration at 10 km downwind is not as important as the fact that it has little effect on the maximum concentration which occurs at 2 or 3 km downwind. This important point must be clear. Stated in another way, the fact that lowering the mixing height increases concentrations at 10 km from 1.6 to 1.7 ug/cu.m., is not as important in urban area as the fact that lowering the mixing height has little effect on the maximum concentration of over 4.0 ug/cu.m. between 2 and 3 km. downwind. As evident from Figure 1, it is the region remote from the source where a shallow mixing depth is most likely to limit dispersion and result in increased pollutant concentrations. It is precisely in this region that the overlap of plumes from multiple sources is most likely to occur. On a regional scale, the maximum concentration from a single source continues to be important but the combined effect from a multitude of overlapping sources is of greater significance than it was on the urban scale. As a consequence definition of mixing depth is of increased importance in regional modelling.

DOWNWIND CONCENTRATION

FOR THREE MIXING DEPTHS

FIGURE 1



Tall Stacks - Effect on Urban and Regional Air Quality

Through the use of stacks more than 300 m tall, it is possible to remove the major part of the pollution problem from an urban area. This strategy was used in Sudbury, Ontario, the site of the 380 m Super Stack. The application of the Sudbury Atmospheric Simulation Model to various pollution control strategies from July 1970 to July 1974, accurately predicted this effect. Experience here has shown the vertical wind profile to be of significance. While the variation of wind velocity with height may be a minor factor in evaluating the impact of 100 - 150 m stacks so familiar in past decades, the increase of wind velocity with altitude is of utmost importance in determining plume rise and resultant downwind concentrations from 300 m stacks. Prior to the installation of the 380 m (1250 ft.) Super Stack, the simulated peak concentrations of SO_2 for 1972 at 121 pphm, which agreed well with the maximum measurement taken in Sudbury for that period of 142 pphm. The simulated air quality levels for 1973 predicted a 66% reduction of these peaks as a result of the Super Stack. The reduction would be greater but for other large sources in the area.

At a distance of 40 km, the simulated concentrations for all sources in and near Sudbury was 12 pphm for the entire period from 1970 to 1973. In other words, the Sudbury Simulation Model predicted that the construction of the Super Stack would have no effect on concentrations more than 40 km distant. This did not quite agree with subsequent measurements. Downwind concentrations at distances greater than 40 km have decreased after the installation of the Super Stack, but at a rate significantly less than that observed in the urban area in which the stack is located. In any event, both from theory and from measurements, we can conclude that while urban air quality may be effectively controlled through the use of tall stacks, the effect of these tall stacks on regional air quality is much smaller. On the regional scale, concentrations of pollutants are more a function of total upwind emissions and, as will be illustrated, the geographic distribution of pollution sources as related to certain atmospheric variables, including regional wind trajectories.

Urban Planning for Environmental Quality

As pointed out by Williams and others (2, 8, 9) land use can be related to pollutant emissions for most categories except large pollutant sources. Thus, urban planners can arrange tracts of residential, commercial, and light industrial land use so as to improve air quality. For example, in Hamilton, Ontario, the fortunate location of heavy industry in the east end of the city is such that frequent southwesterly winds carry pollutant emissions out over Lake Ontario, just offshore of the residential communities of Burlington and Oakville, (See Map II "Location of Major SO_2 Sources"). Geography and meteorology rarely offer the planner such an opportunity. The effectiveness of this kind of control is more often offset by the atmospheric transport of pollutants from large sources. Williams, Ozolins, Sadler, and Farmer (8) have shown the wide range of "local" SO_2 emissions which can result in the same mean air quality. The benefical effects of locating 100 meters of open space around a sewage treatment plant may be offset by the plume of a sludge incinerator which produces maximum odours at a distance of 1000 meters. Some very large sources, such as power plants, have less effect on adjoining residential areas than on high rise apartments at a distance of 10 or 20 kilometers.

The limitation of the assumption that land use is correlated with pollutant emissions and emissions in turn to mean annual values of urban air quality is best illustrated in the case of Sudbury, Ontario, where SO_2 emissions are among the highest in North America, while mean annual air quality levels are not unlike Toronto or Hamilton. The total SO_2 emissions in Sudbury, Toronto, and Hamilton are in the ratio of 50 to 7 to 1. However, the mean annual concentrations of SO_2 in all three of these cities are similar; they all range between 1 and 2 pphm. This comparison illustrates that pollutant emissions are only one of the factors which need to be considered in controlling air quality.

The attempts of Williams and others to relate air quality to land use planning will be far more successful on a regional scale than they have been in the urban atmosphere. The cumulative emissions from varied land use along a regional trajectory will be more nearly correlated to downwind air quality that attempts to relate land use within an area to air quality in that same area. The factors which tend to limit Williams' assumptions on the urban scale, i.e. tall stacks and atmospheric transport terms, are of a different order of importance on a regional scale. The effect of a tall stack on pollutant concentrations 50 km downwind can be assumed to be very small. The transport term can be accounted for by summing pollutant emissions from varied land use along a regional velocity trajectory.

Urban Planning and Regional Environmental Quality - An Example

Once a meteorologist has defined critical trajectories, the atmospheric systems engineer can simulate the effect of existing sources on regional air quality. Together with the urban planner, this team can then consider future urban plans and sites of major pollution sources so as to maintain quality air. Simulated air quality for both present and future source configurations may be compared with desired air quality.

Consider, for example, a proposal to locate a fossil fuel power generating station mid-way between Toronto and Hamilton. Locating a 6000 Mw plant with a 300 m stack on the lakeshore, 25 km upwind of the receptor point shown in table 1, would result in a total SO_2 concentration of 46 pphm in Hamilton exceeding the Ontario criteria for hourly SO_2 concentrations of 25 pphm.

While not undesirable in itself, a concentration of 22 pphm from a 6000 Mw power station when added to the pollution accumulated from multiple sources along a trajectory from Toronto to Hamilton will produce an undesirable effect. Moving the location of the power plant as little as 5 km off the northeast to southwest trajectory would reduce the contribution of this plant to result in a total concentration near the criterion of 25 pphm.

Conclusion

Urban growth on a regional scale poses a challenge to a wide spectrum of professions which includes meteorologists, engineers, and urban planners. All of us must realize that the experience we have gained in the past will have to be examined in light of industrialization and urbanization on a larger scale than we have before known.

At the present time more than four million pounds of SO_2 are emitted into the Ontario atmosphere each year. The potential damage from this amount of pollutant has been estimated (10) as more than 800 million dollars. In cities such as Toronto, urban simulation models have been successfully used in the development of efficient strategies to control SO_2 at a small fraction of the cost of the potential damage. A new challenge lies ahead as problems confront us in regional atmospheric modeling, such as the description and modeling of wind trajectories and thermal gradients in three dimensions, which have assumed added importance. The application of atmospheric simulation models to the management of regional air quality provides an opportunity for the meteorologist, atmospheric systems engineer, and urban planner to work together in a new and meaningful way.

Acknowledgement

The simulation models and support systems reported on here have been developed by the staff of the Atmospheric Systems Group. Particular thanks go to Ken Trent for his diagnosis of the effects of mixing depth and for his work in developing and verifying the Sudbury Simulation Model. Implimentation and updating of the inventory support systems was performed by the District Office staff of the Air Management Branch.

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Chapter 22

THE UTILIZATION OF AN URBAN AIR POLLUTION MODEL IN AIR MANAGEMENT

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Introduction

A multiple-source urban diffusion model was developed for Metropolitan Toronto in 1971 and has been in use by Ontario's Ministry of the Environment, Air Management Branch, for the past year. The model is an adaptation of the regional model originally designed for Connecticut and described in a report by Hilst.[1] Modifications were made in the development of the model for Metropolitan Toronto which were described in a paper by Bowne, Boyer et al.[2]

This paper will discuss the emission inventory system, the meteorological input, the verification of the model, and the applications of it which have been carried out by the Ontario air pollution control authority.

Emission Inventory

A comprehensive emission inventory was completed for the Metropolitan Toronto area and, later, for Hamilton, Ontario. Some 10,000 man-hours were required to obtain an inventory of five pollutants for Toronto. The pollutant inventory included sources of sulphur dioxide, nitrogen oxides, particulate, carbon monoxide, and hydrocarbons. The Hamilton inventory was completed with less than 3,000 man-hours, in part because there were fewer sources, in part because the experience gained in the Toronto inventory made possible a more efficient use of resources.

Inventory field work can be greatly reduced using the following guidelines:

1. Detailed surveys may be restricted to those sources emitting more than 1000 lbs/day of SO_2 or NO_2 pollutant, or 300 lbs/day of particulate.
2. The detailed emission survey for Toronto provided the relationship by which emissions from smaller commercial or industrial sources may now be estimated as follows:
   - (a) 75 lbs SO_2/year/employee, or
   - (b) between 1000 and 3000 lbs/SO_2/year/acre of commercial or industrial land use, or
   - (c) between 0.1 and 0.3 lbs. SO_2/square feet/yr. of commercial or industrial floor space heated by burning fuel oil.

It should be emphasized that these guidelines apply only to small firms.

The large amount of emission data were processed and stored in a computerized information system.[3] This system may generate a variety of reports from the data base, provides the emission values for the Simulation Model, and has the design capability for being readily updated or changed for the testing of control strategies.

The sources were classified into three types; major sources were treated as point sources with detailed information obtained regarding rate of emissions, seasonal and diurnal variability, temperatures and velocity of the flue gas at point of emission, stack dimensions which are required for the computation of the plume rise, and effective stack height which is an input in the dispersion formula. The criterion for a point source is the emission in excess of 1000 pounds per day of any one pollutant. Lesser sources, such as homes and commercial establishments, were surveyed in groups, with a single emission being derived for an entire area. Automotive emissions were also included as area sources, except for major transportation routes which, with traffic counts, became classified as line sources.

A summary of emissions by source and type, giving the weights emitted per year and the percentages of the total for each of the five pollutants, are shown in Table 1, "Emission Summary - By Pollutant" - Metropolitan Toronto, and Table 2, "Emission Summary - by Pollutant" - Metropolitan Hamilton.

The greatest sources of sulphur dioxide and nitrogen oxides are the generating stations. Suspended particulate matter was emitted by a more equal distribution of sources, except in Hamilton where most of the particulate emissions originate at the steel mills. Automobiles are the principal sources of carbon monoxide and hydrocarbons. Although the automobile is shown to be the greatest source of pollution, with the emission of over 800 million pounds of carbon monoxide in Toronto alone, it should be pointed out that the relative differences in the severity of effects must be taken into account in rating a source or class of sources.

Meteorological Input

The Air Quality Model produces computations of the hourly average concentrations of each of the five pollutants for each hour of the day for a location defined by the grid square based on the Universal Transverse Mercator System.

The input consists of the source inventory, the windfield and other meteorological data. The input data is defined for each hour of the day for which the air quality concentrations are desired to be computed. Options are available to delete specific sources, modify any source, or modify an entire class of sources.

In simulating meteorological conditions for the purpose of testing abatement strategies, it is generally acknowledged that those limiting meteorological conditions which produce peak concentrations should be used, the rationale for this being that if the strategy is effective under such limiting conditions, then it will also be effective under all less severe conditions.

Listed in Table III, "Limiting Meteorological Conditions, Toronto, Ontario", are those meteorological conditions which occurred simultaneously with the upper five percentile of measured concentrations of SO_2 at the College Street sampler in midtown Toronto for any given wind direction.

It is interesting to note that for the highest measured concentrations, limiting meteorological conditions occur with moderate wind speeds in the range of 6 - 8 m/s. This may be a reflection of the fact that in Toronto the higher concentrations of SO_2 are due to emissions from elevated sources which require a moderate wind to bring the plumes down to near ground level.

For offshore winds, concentrations, while lower, tend to peak at lower wind speeds (2 - 3 m/s). This is probably a reflection of the fact that with offshore winds most of the sources are low elevation sources, such as residences and commercial institutions, which would produce peak concentrations with low wind speeds and low mixing heights.

The importance of the windfield in any urban model is difficult to exaggerate. As described by Hilst[1] and others[2], urban air quality simulations are most sensitive to errors in wind direction. Though many urban windfield models have been proposed, few can be made to operate with the accuracy required to explain the variability in pollutant dispersion which we know to exist from analysis of pollutant measurements.

Verification of a numerical heat island-lake breeze model by comparison with hand analysis of streamlines has shown that, in many instances, this model[4] did not provide the accuracy required for the purpose of verifying air quality predictions.

Over the past two years, continuous operational use of various windfield options has favoured a numerical model based on a simple distance weighting function[5] applied to the reported wind velocity measurements. This model has been used with success in the Toronto area, where lake breezes are an important part of pollutant dispersion. It has also been used with initial success in the urban model for Hamilton, Ontario, where both lake breezes and orographic influences markedly affect the windfield. In this latter case, the large number of meteorological stations (five) in the vicinity of the lakeshore and escarpment make it possible to describe the effect of local influences in the windfield, if not to explain the mechanisms involved.

The windfield is obtained by determining the wind velocity vector for each grid point, utilizing a weighting or interpolation method according to equation 1:

$$u(i,j) = \frac{\sum_{1}^{N} W(K) \quad u(K)}{\sum_{1}^{N} W(K)} \qquad (1)$$

where u is the x component of the wind velocity at grid location i,j.

K is the number of a wind reporting station.

N is the total number of wind reporting stations.

W(K) is weighting function for Station K. A different W is computed for each grid location for each reporting station by equations 2 and 3. A similar equation may be written for v, the y component of the wind velocity.

The method is based on the distance between the grid point and the locations of the measured wind velocities. The nearest measuring station to the grid point receives the highest weighting in the computation of the wind vectors:

$$W(K) = \exp\left[- \frac{(XK)^2}{SX(K)} - \frac{(YK)^2}{SY} \right] \qquad (2)$$

where XK and YK are distances as shown in Fig. 1. The reference system is oriented in the direction of the observed wind. The (XK, YK) reference system, as shown in Fig. 1, is oriented in the direction of the observed wind, with the origin at the weather station (K), and MPH(K) is the wind speed at Station K. Where SX(K) is defined by equation 3:

$$SX(K) = SY\left(1 + \frac{MPH(K)}{12}\right) \qquad (3)$$

SY is assigned a value between 40 and 70, depending upon the density of wind reporting stations. The larger the number of stations, the lower should be the value of SY.

It is evident from the equations above that for any set of wind reports SY will determine the sensitivity of the final analysis to the distance between a grid point and reporting stations. For low values of SY, the analyzed wind velocity at any grid point will be more dependent upon nearby stations. Also, since SX is always greater than SY (except where MPH = 0), the final analysis will be more dependent upon downwind distance (XK) than on crosswind distance (YK).

Reliability

A most stringent test of any simulation model is the degree to which the model can reproduce real-life conditions. The atmospheric models used in Ontario attempt to reproduce variations in air quality for space scales as small as one kilometer, for time periods as short as one hour. For this "space-time" scale, 70 per cent of the predictions are within a factor of two of the measured values.[2]

Fortunately, it is not required to know air quality variations to the nearest hour for most planning purposes. If we consider the frequency of predicted air concentrations over a period of days, the model will produce a more reliable simulation. For such time periods, the frequency of predicted concentrations will be within 10 per cent of those which have been measured. An example of predicted and measured concentrations of SO_2 in the centre of Toronto is shown in Fig. 2, "Frequency of Measured and Predicted SO_2 Concentrations". This summary includes 14 selected days between February and August, 1971.

Scoring of Results

If the goal of air pollution control is defined in terms of legislated air quality levels, the starting point of any control plan is logically the existing air quality. The frequency of air quality values consistent with desired goals can be inferred from specified annual averages and maxima.[6] The air quality objective, shown in Fig. 3, was estimated from Ontario's desired goals for SO_2 which set the annual mean at 2 p.p.h.m. and the hourly maximum at 25 p.p.h.m.

Specification of the criteria by which present or predicted air quality levels are scored will, in large part, determine the characteristics of the system design.[7] The lack of favour which certain air pollution simulation models have incurred may well be due to the fact that the measures chosen to depict simulated air quality were less than crucial.

Of prime importance in pollution control are those peak concentrations which occur infrequently. Those concentrations which are exceeded only once a year, or only 1 per cent of each year, are usually more important than those concentrations near the annual average which occur thousands of hours each year. This is particularly true in those locations where a single large source is responsible for most of the pollutant emissions. Under such conditions, the annual average may be low while, on certain days, concentrations may be excessive.

In recent years, it has been customary to present measured or predicted concentrations of air quality for an entire spectrum of occurrences. Such a presentation is shown in Fig. 3, "Frequency of SO_2 Concentrations".

Typical Simulation - Air Quality 1975

Very often the evaluation of a particular plan will point out both the deficiencies of that specific plan, as well as the problem areas which must be considered in more detail.

Typical examples of simulations which have been completed during the past year include prediction of the air quality in Toronto in 1975, after completion of all existing pollution abatement programs.

Preparation of the simulated air quality for 1975 pin-pointed remaining problem areas. The simulation showed that, while the air quality will be greatly improved on the average, there will be certain periods when a combination of circumstances will result in air quality not markedly different than it was during the base year of 1969 - 1970.

The highest concentrations of SO_2 in Toronto presently occur, and will continue to occur, when the plumes of the Hearn and Lakeview Power Generating Stations are over the city. One such condition occurs with a strong southwesterly wind.

Various abatement strategies aimed at reducing sulphur dioxide emissions by the year 1975 were to be scored. More than twenty different sets of meteorological conditions were specified as the basis for testing the proposed 1975 strategies. These are listed under "Onshore Winds" in Table III. Of these, the simulation for southwesterly winds will serve as an example of the technique followed.

As the first step, pollutant emissions and meteorological conditions for the winter of the base year (1969 - 1970) were reproduced. Those atmospheric conditions which occurred simultaneously with the upper five percentile of SO_2 concentrations during southwest winds were tabulated. This sample included 35 hours which represents an annual frequency of 0.4 per cent.

The results of the first attempt to simulate air quality for the base year are shown in Fig. 4. This simulation of the recent past indicates that the College Street sampler would have been near the centre of an elongated area of high SO_2 concentrations.

The predicted value for the sampler location was 20 p.p.h.m. This is slightly higher than the measured concentrations of 18 p.p.h.m. known to have occurred with the specified meteorological conditions. The predicted and measured air quality values are marked in Fig. 3, "Frequency of SO_2 Concentrations". The simulated concentrations are based on the limiting meteorological conditions shown in Table III for winds from 232 degrees.

A second simulation was then set up by modifying the emission inventory to reflect the various strategies for reducing SO_2 levels. These included:

1. Restricting fuels to a sulphur content of 1.5 per cent.
2. Converting forty large sources of SO_2 to natural gas.
3. Extensive modification to the structure and operation of the two power generating stations.

The predicted air quality in the year 1975 is shown in Fig. 5, "Predicted SO_2 Concentrations for 1975 for Limiting Meteorological Conditions".

It may be noted from Fig. 5 that pollution patterns were not markedly changed by the 1975 strategies, although pollution levels were predicted to be somewhat less. For the College Street sampler location, the predicted air quality in 1975 would be 14 p.p.h.m. This is noted in Fig. 2 as about 50 per cent of the reduction required to meet the air quality objective of 10 p.p.h.m. at an annual frequency of 0.4 per cent (see * marked predicted 1975).

In summary, measurements indicate that for the College Street location, SO_2 concentrations exceed the air quality objective. At the 0.4 percentile, measured SO_2 concentrations of 18 p.p.h.m. exceed the desired goal by 8 p.p.h.m. (see Fig. 3). Predictions of SO_2 for 1975, based on simulated emissions and specified atmospheric conditions, show that the proposed strategies will reduce SO_2 levels to 14 p.p.h.m., or 50 per cent of the required reduction.

Simulation of Carbon Monoxide Concentrations Resulting from Automotive Emissions

An attempt was made to reproduce the existing air quality as it is affected by auto emissions. First attempts failed because it was not understood that emissions from autos spread out in a thin layer near the ground. This is very different from the experience with the dispersion of pollutants from tall industrial stacks.

By limiting the mixing of auto pollutants to a height of 30 meters, we were able to reproduce the observed variation of CO concentrations. The simulated concentrations, shown in Fig. 6, are well within the criterion specified in Ontario Regulations.

However, as a result of these findings, it is now felt that the auto may be a more important source of nitrogen oxides as measured near ground level. While the emissions of nitrogen oxides from autos are small as compared with other sources, if these emissions are spread in a shallow layer as is carbon monoxide, then the contribution of these emissions to air concentrations of nitrogen oxides near the ground will be far greater than has been expected in the past. This problem is now under study.

Toronto District Heating Study

The Air Quality Model has been used to evaluate air pollution resulting from various district heating schemes being considered by the City of Toronto in their District Heating Study. Other factors, such as cost, heat demand, aesthetics, and size form the overall study and combine with the air pollution modeling results in the overall considerations of the optimum central heating schemes.

Among the various alternative designs considered were a group of heating plants for the core area of Metropolitan Toronto, as compared with expansion of existing heating systems. Simulated air quality shows that both designs would exceed Ontario Criteria. The district heating plant option would result in a marked improvement over simple expansion of "as is" heating units. Other alternatives are now under study.

Urban Planning

District heating plans for the year 1989 required consideration to be given to urban growth and its impact on the atmospheric environment. Projections were available in terms of land use, population, and employment. In order to relate this to pollutant emissions, a simple statistical study was made of the relationship between land use and SO_2 emissions. This inter-relationship is shown graphically in Fig. 7.

Sulphur oxide emissions range from a few hundred pounds per acre per year in residential areas to 1000 to 2000 pounds per acre per year for commercial areas of Toronto. Industrial areas range anywhere from a few thousand pounds per acre per year to 50,000 pounds per acre per year.

Further study has shown that pollutant emissions from industrial areas are more nearly correlated with employment than with land use, commercial emissions depend both on land-use acreage and on employment, while residential and apartment emissions are best estimated on the basis of population density. SO_2 emission, as a function of employees in commercial buildings, is shown in Fig. 8. Most firms will emit about 75 pounds SO_2 per employee per year. With this knowledge, it was possible to estimate the emissions of SO_2 in 1989, based upon projections of land use, population, and employment.

The techniques described above cannot be used to predict emissions from large pollutant sources, such as power plants, refineries, steel mills, smelters, and so on. The impact of these large sources is best handled by specifying the location of the source and estimating the emissions on the basis of estimates of product output.

Specifying urban plans in terms of land use and population density is complicated by the fact that pollutants are transported through the atmosphere from one land-use designation to adjoining ones. Pollution from large sources may be transported over many miles.[8] The prospect of using open space to separate pollution sources from residential areas may work well for the small industrial sources, but is out of the question for large sources.

Air Quality Planning

The components of an atmospheric environment system are shown in Fig. 9. At the heart of this system is the present air quality. To illustrate the application of this system, consider the evaluation of the strategy to reduce SO_2 levels in Toronto, which has previously been described.

1. START with present air quality.
2. SCORE present air quality.
3. Favourable Options? No. SO_2 levels greater than air quality objective (18 vs 10 p.p.h.m. - see Fig. 3).
4. "TEST Next Source Control Plan"; in the example of Toronto 1975, this source control plan included various sulphur oxide restrictions.
5. "Manipulate Emission Inventory". Base-year inventory is modified to simulate SO_2 emissions in 1975 by deleting sources, modifying source emissions, or modifying emissions from an entire class of sources to reflect proposed fuel sulphur restriction.
6. "Air Quality Simulation Model". Specify appropriate atmospheric conditions; predict air quality for 1975; go back to Score.
7. SCORE predictions.
8. Favourable Options? No. SO_2 levels are predicted to be above the goal (14 vs 10 p.p.h.m.)

Since no other source control plan is to be considered, this is the end point of the example. This process may be repeated until one or more strategies result in favourable options, after which one of the options will be selected as the optimum plan to be implemented.

TABLE I

AIR QUALITY MODEL FOR METROPOLITAN TORONTO

EMISSION SUMMARY - BY POLLUTANT

MILLIONS OF LBS. EMITTED PER YEAR

SOURCE TYPE	SO_2	PARTICULATE	NOX	CO	HC
R.L. HEARN G.S.	34.64	0.62	26.44	0.29	0.12
LAKEVIEW G.S.	348.28	5.94	80.19	2.00	0.81
MUNICIPAL INCINERATORS	0.55	12.13	1.35	3.28	0.16
INDUSTRIAL SOURCES	23.25	12.08	17.64	4.89	43.64
AUTOS	3.49	4.65	43.65	827.36	126.42
RAILROADS	0.43	1.08	2.19	0.59	1.33
SHIPPING	0.90	0.41	0.66	0.24	0.32
AIRCRAFT	0.24	1.18	1.14	2.21	10.61
HEATING - RESIDENTIAL	19.82	2.49	5.91	0.52	0.76
HEATING - APARTMENTS	10.73	3.99	5.68	3.88	0.84
HEATING - SCHOOLS & UNIV.	8.29	0.83	2.69	0.29	0.11
HEATING - PUBL. & COM. BLDGS.	14.40	2.83	10.77	0.74	0.34
SMALL INDUSTRIES	7.19	0.83	2.54	0.23	0.10
INCINERATION	0.07	1.16	0.26	1.76	0.11
TOTAL 1757.56	472.28	50.22	201.11	848.28	185.67

TABLE II

AIR QUALITY MODEL FOR HAMILTON

EMISSION SUMMARY - BY POLLUTANT

MILLIONS OF LBS. EMITTED PER YEAR

SOURCE TYPE	SO_2	PARTICULATE	NOX	CO	HC
INDUSTRIAL SOURCES	62.20	50.43	80.65	7.49	25.15
AUTOS	0.47	0.63	5.88	133.20	18.29
RAILROADS	0.09	0.24	0.49	0.13	0.30
SHIPPING	2.91	0.29	0.64	0.07	0.14
HEATING - RESIDENTIAL	3.15	0.40	0.97	0.08	0.12
HEATING - APARTMENTS	0.44	0.24	0.35	0.23	0.05
HEATING - SCHOOLS & UNIV.	1.88	0.31	0.74	0.15	0.05
HEATING - PUBL. & COM. BLDGS.	1.84	0.24	0.95	0.05	0.03
SMALL INDUSTRIES	0.40	0.06	0.26	0.01	0.01
INCINERATION	0.01	0.08	0.04	0.22	0.01
TOTAL 403.06	73.39	52.92	90.97	141.63	44.15

TABLE III

LIMITING METEOROLOGICAL CONDITIONS - TORONTO, ONTARIO

OFFSHORE WINDS, SEASON - WINTER							ONSHORE WINDS, SEASON - WINTER						
Direction	Speed m/sec.	Tor.Int'l Airp.-°F.	Bloor St.-°F.	Stability	Mixing Height Meters	Meas. Concent. pphm	Direction	Speed m/sec	Tor.Int'l Airp.-°F.	Bloor St.-°F.	Stability	Mixing Height Meters	Meas. Concen. pphm
056	0.5	14	18	5	100	12	136	5.8	14	18	4	1000	25
056	2.2	14	18	5	300		144	3.6	14	18	4	1000	
048	2.2	15	18	5	300	11	152	4.0	14	18	4	1200	
040	2.2	15	18	5	300		157	4.0	14	18	4	1200	20
032	2.2	14	18	5	400		160	4.0	14	18	3	1500	
024	3.6	14	18	5	400	11	168	4.0	14	18	3	1500	
016	3.1	15	18	3	500		176	5.4	15	18	4	1200	
008	3.1	16	20	3	500		180	6.7	17	20	4	1200	30
240	3.1	16	21	3	500		184	8.0	19	21	4	1200	
248	3.1	17	22	3	600	14	192	7.2	19	22	4	1200	
256	3.1	19	24	2	600		200	6.7	20	24	4	1200	22
264	3.1	19	24	2	600		208	6.7	21	24	4	1200	
272	3.1	19	23	2	600	09	216	6.7	19	23	4	1200	
280	3.1	18	22	3	600		224	6.7	18	22	4	1200	18
288	2.2	17	21	3	600		232	6.7	17	21	4	1200	
296	2.2	13	18	3	500	08	128	4.9	13	18	4	1200	
304	2.2	13	18	3	500		120	6.7	14	18	4	1200	
312	2.2	14	18	4	400	11	112	2.2	13	18	4	1200	20
320	2.2	14	18	5	400		104	4.5	14	18	4	1000	
328	2.2	14	18	5	400		096	4.5	13	18	4	700	
336	2.2	14	18	5	300	12	088	2.2	13	18	5	400	07
344	2.2	14	19	5	300		080	2.2	14	19	5	400	
352	2.2	15	19	5	300		072	2.2	15	19	5	400	
360	2.2	14	19	5	300	12	064	2.2	14	19	5	400	09

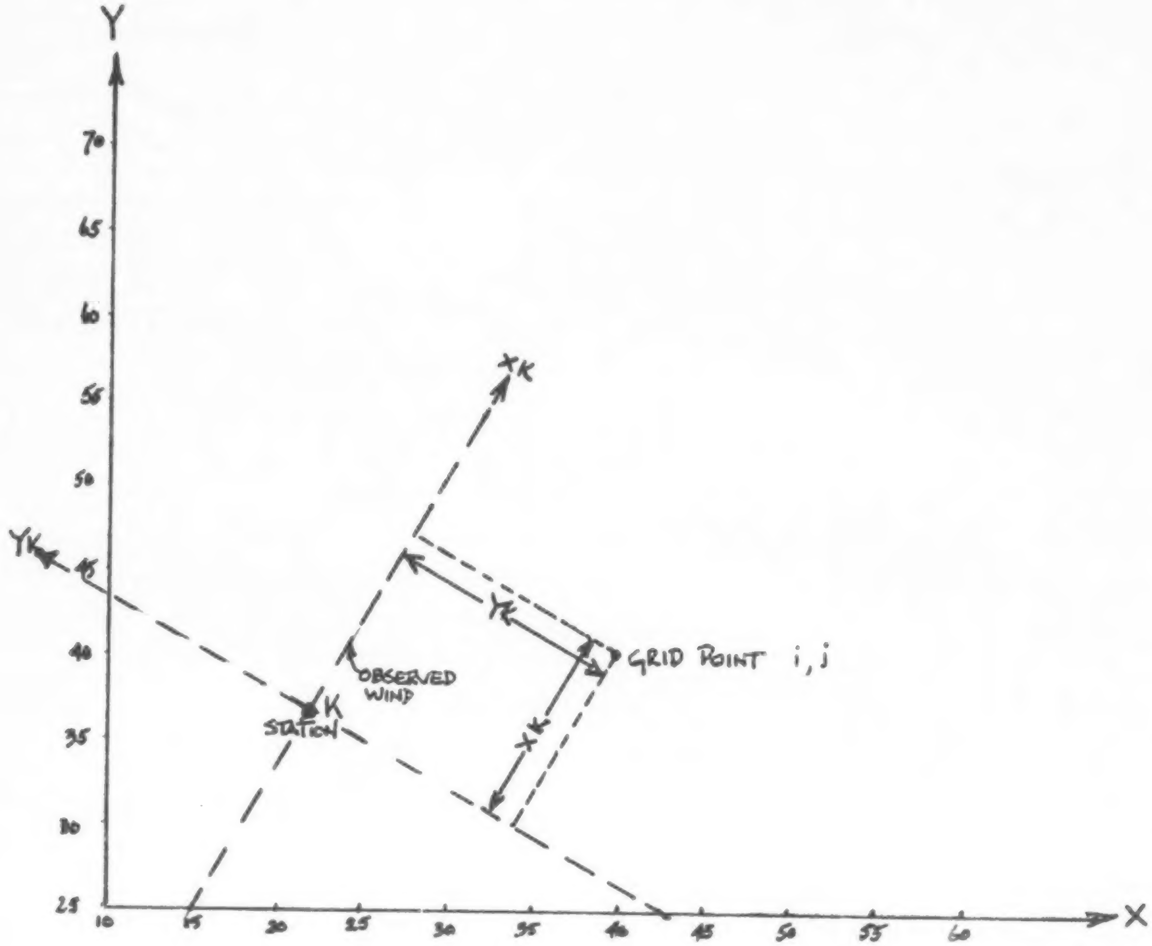

Y
70
65
60
55
50
45
40
35
30
25
10
15
20
25
30
35
40
45
50
55
60
X
XK
YK
YK
XK
OBSERVED WIND
K
STATION
GRID POINT i, j

Fig. 1 - WINDFIELD GRID SYSTEM

FREQUENCY OF MEASURED AND PREDICTED SO_2 CONCENTRATIONS

COLLEGE ST. SAMPLER

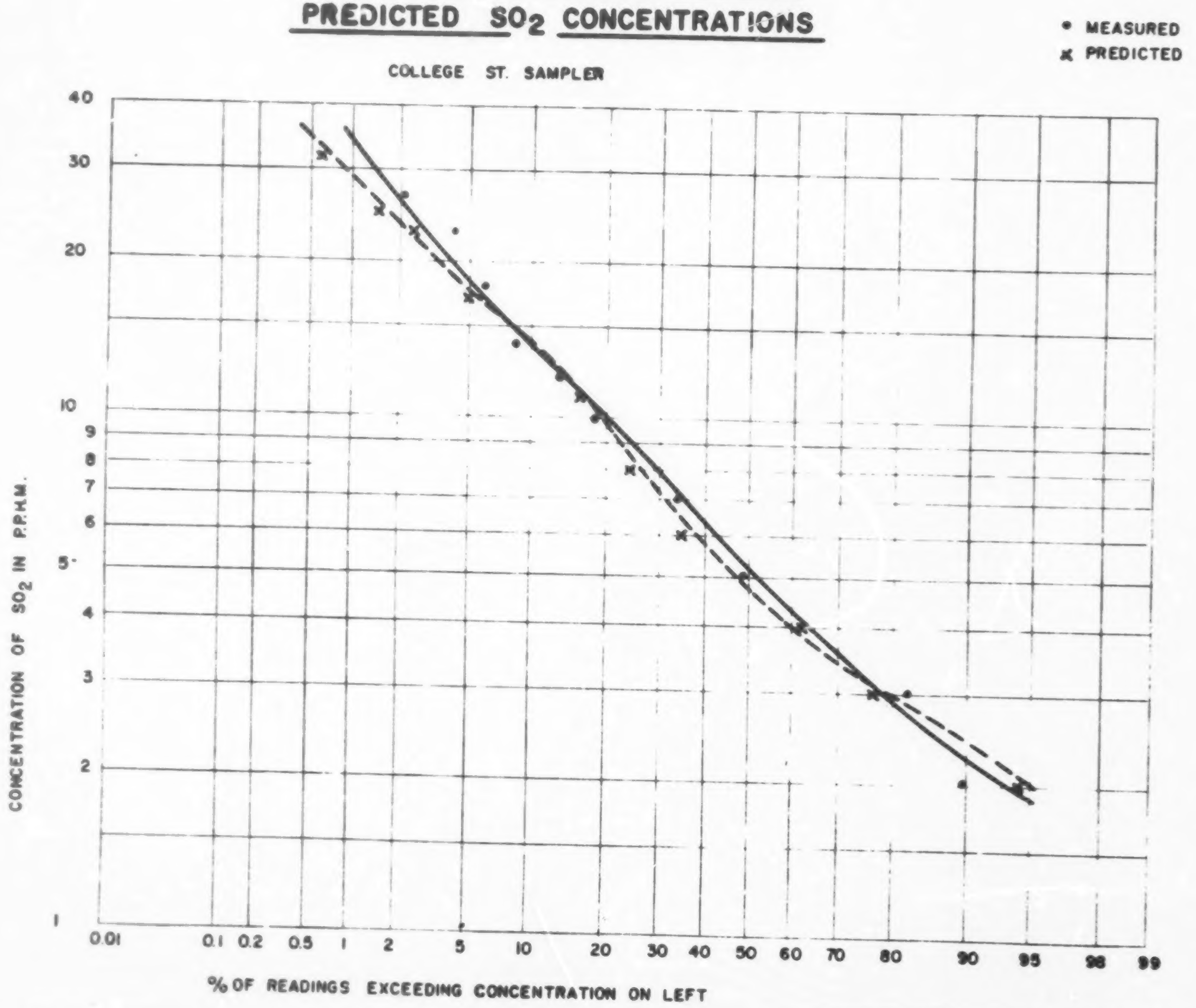


FIG.: 3 - FREQUENCY OF SO 2 CONCENTRATIONS

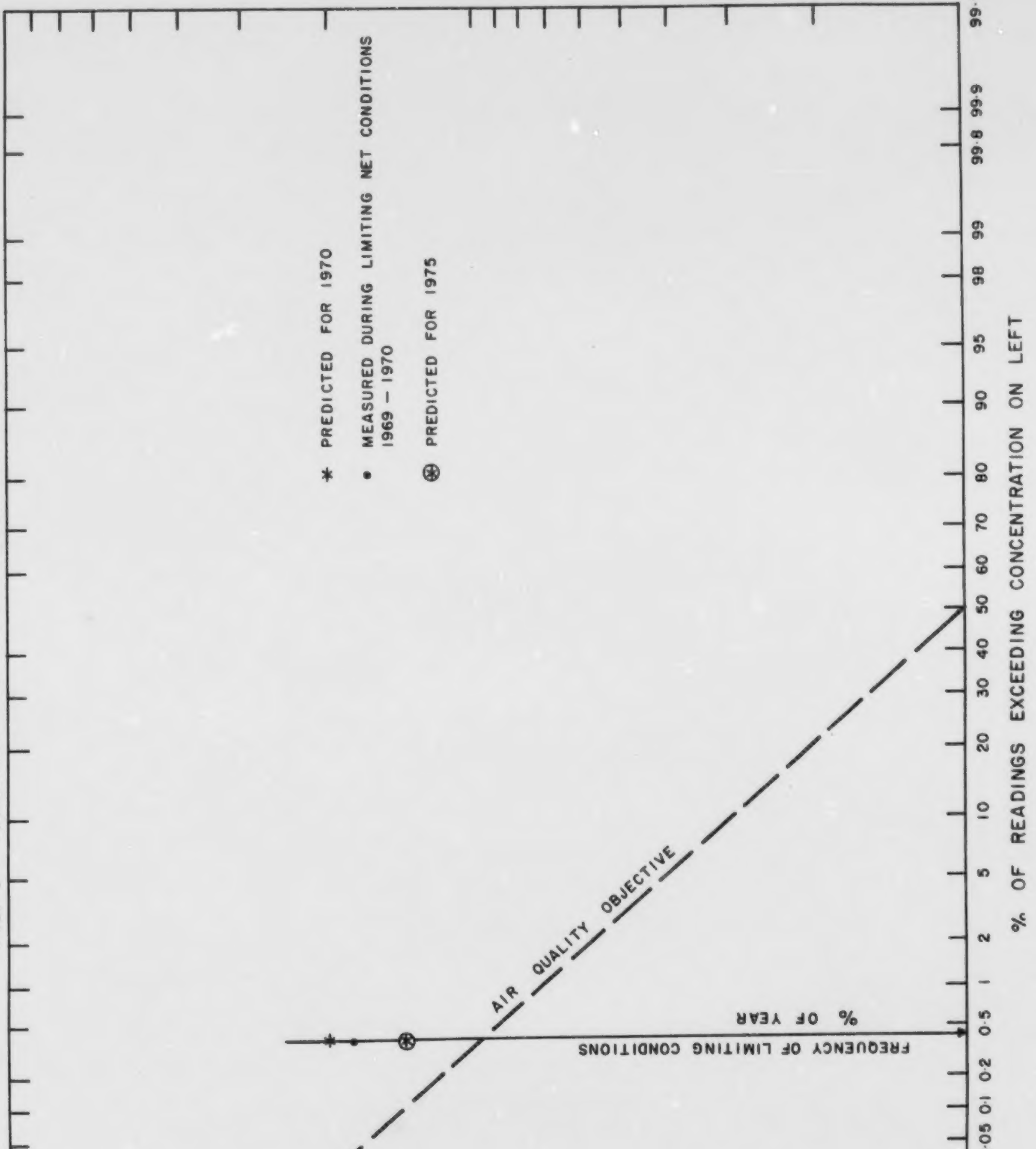


FIGURE : 4 PREDICTED SO_2 CONCENTRATIONS (p.p.h.m.) FOR BASE YEAR EMISSIONS AND LIMITING METEOROLOGICAL CONDITIONS

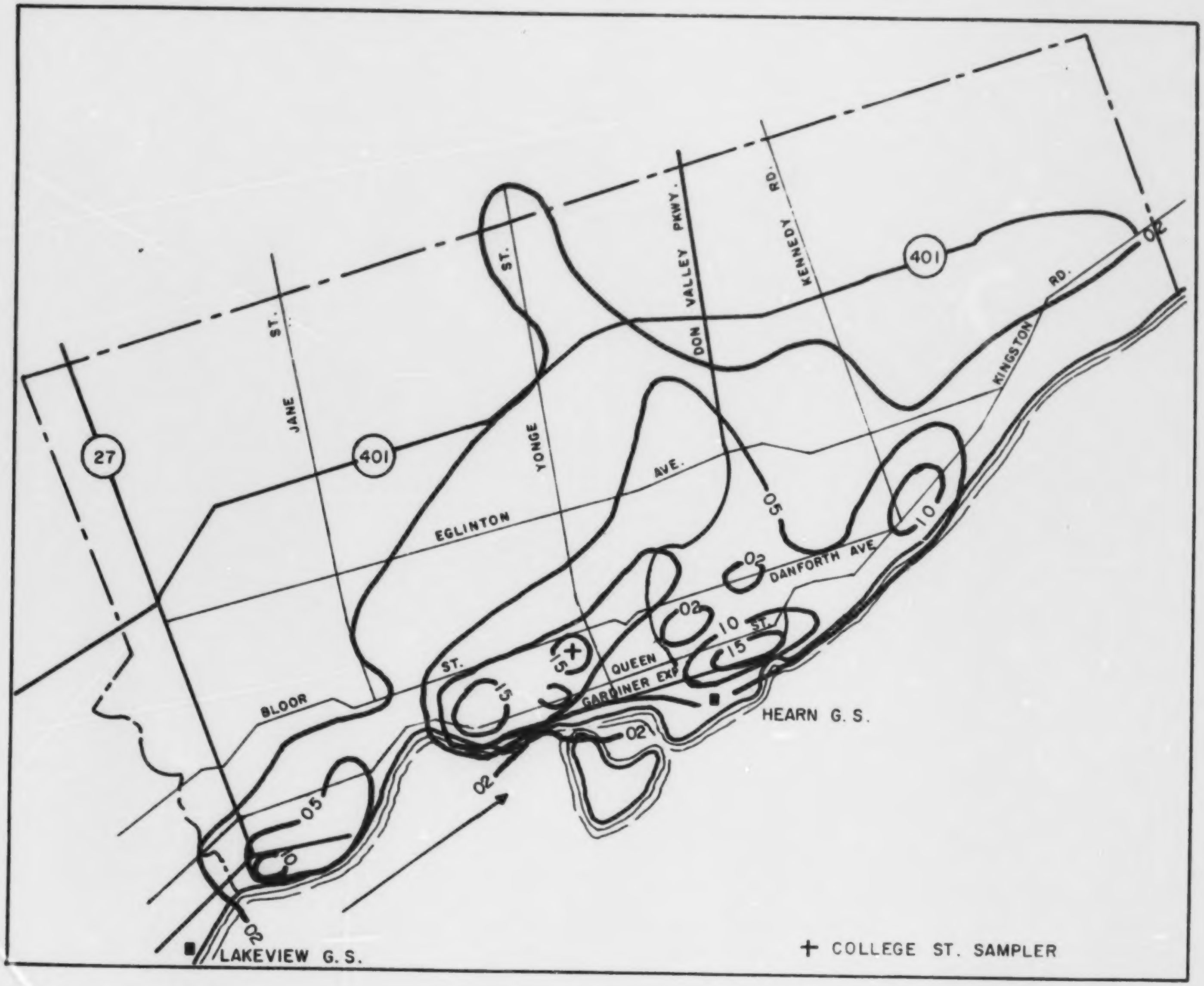

27
401
401
JANE ST.
YONGE ST.
DON VALLEY PKWY.
KENNEDY RD.
KINGSTON RD.
EGLINTON AVE.
DANFORTH AVE
BLOOR ST.
QUEEN ST.
GARDINER EXP.
HEARN G. S.
LAKEVIEW G. S.
+ COLLEGE ST. SAMPLER
02
05
10
15
15
15
10
05
02
02
02
02
02
05
10
02

FIGURE : 5 PREDICTED SO_2 CONCENTRATIONS (p.p.h.m.) FOR 1975 FOR LIMITING METEOROLOGICAL CONDITIONS

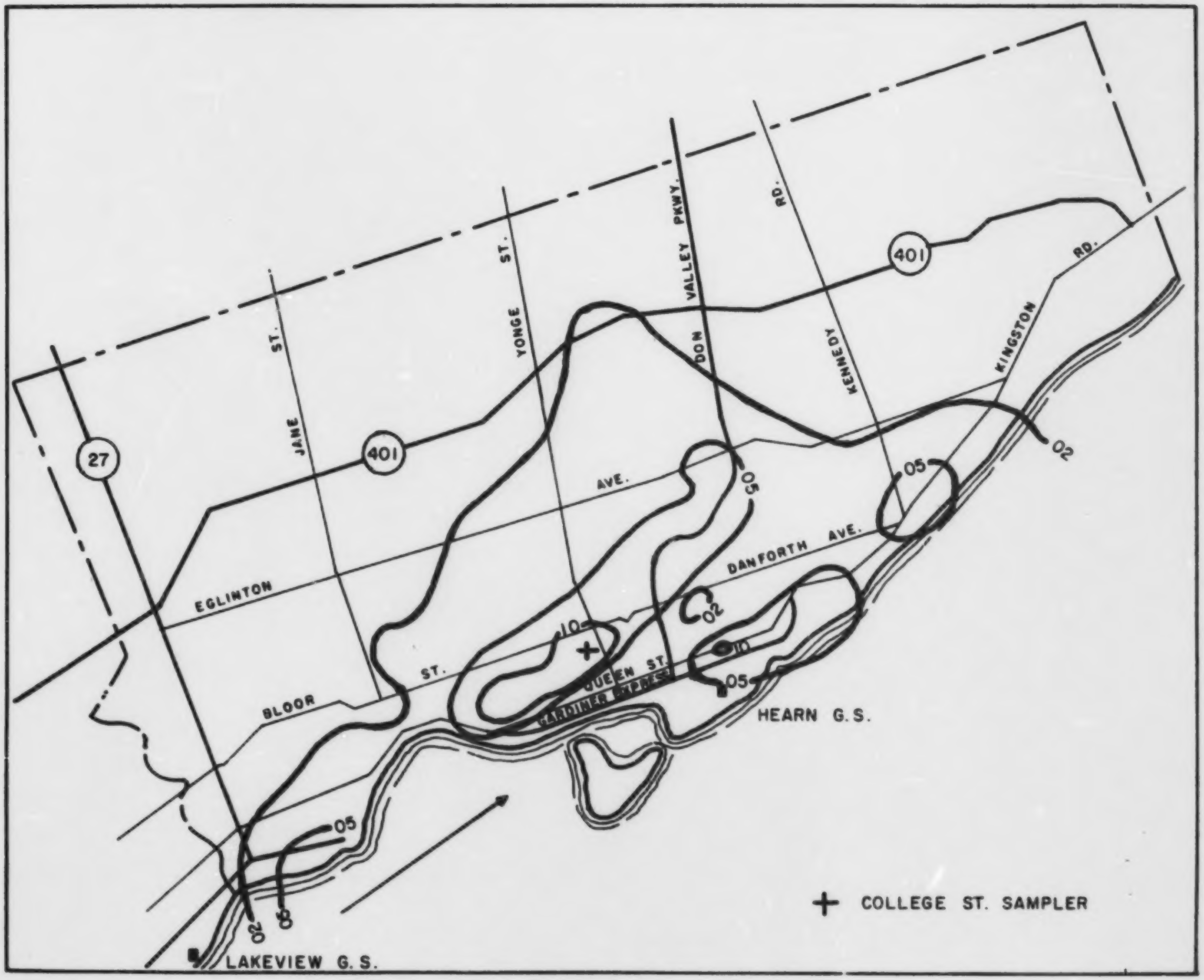
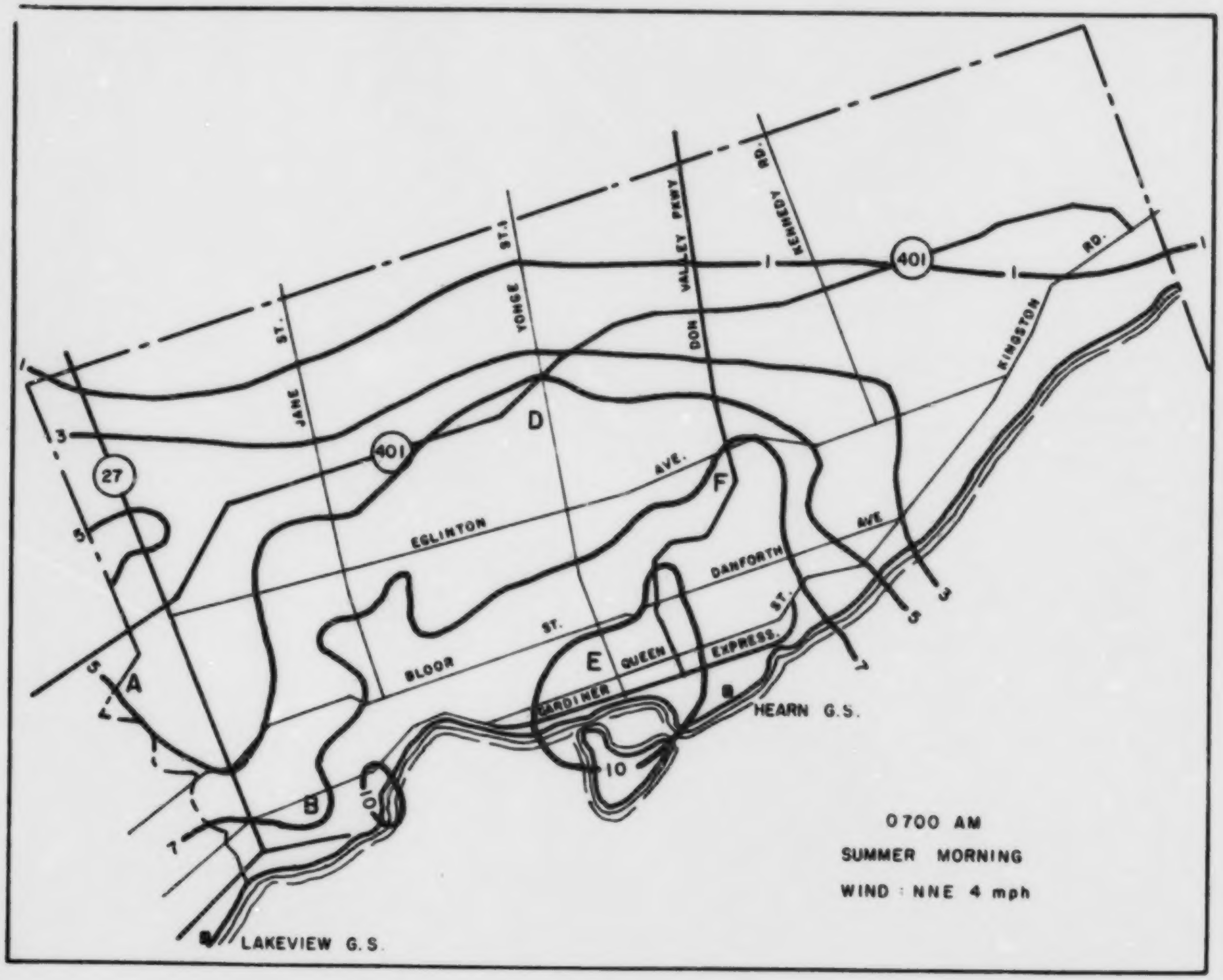

27
401
401
JANE ST.
YONGE ST.
DON VALLEY PKWY.
KENNEDY RD.
KINGSTON RD.
EGLINTON AVE.
DANFORTH AVE.
BLOOR ST.
QUEEN ST.
GARDINER EXPRESS
HEARN G.S.
LAKEVIEW G.S.
02
05
10
05
02
10
05
05
02
05
08
02
+ COLLEGE ST. SAMPLER

FIGURE : 6 CARBON MONOXIDE PREDICTED CONCENTRATIONS (p.p.m.)


JANE ST.
YONGE ST.
DON VALLEY PKWY
KENNEDY RD.
KINGSTON RD.
401
27
EGLINTON AVE.
DANFORTH AVE.
BLOOR ST.
QUEEN ST.
GARDINER EXPRESS.
A
B
D
E
F
1
3
5
7
10
HEARN G.S.
LAKEVIEW G.S.

0700 AM
SUMMER MORNING
WIND : NNE 4 mph

GROUND LEVEL PREDICTIONS

STATION		CONCENTRATION (ppm) OBSERVED	CONCENTRATION (ppm) PREDICTED
A	=	6	6·3
B	=	7	7·3
D	=	5	7·5
E	=	10	13·8
F	=	8	9·0

FIGURE : 7 — SULPHUR OXIDE EMISSIONS BY LAND USE

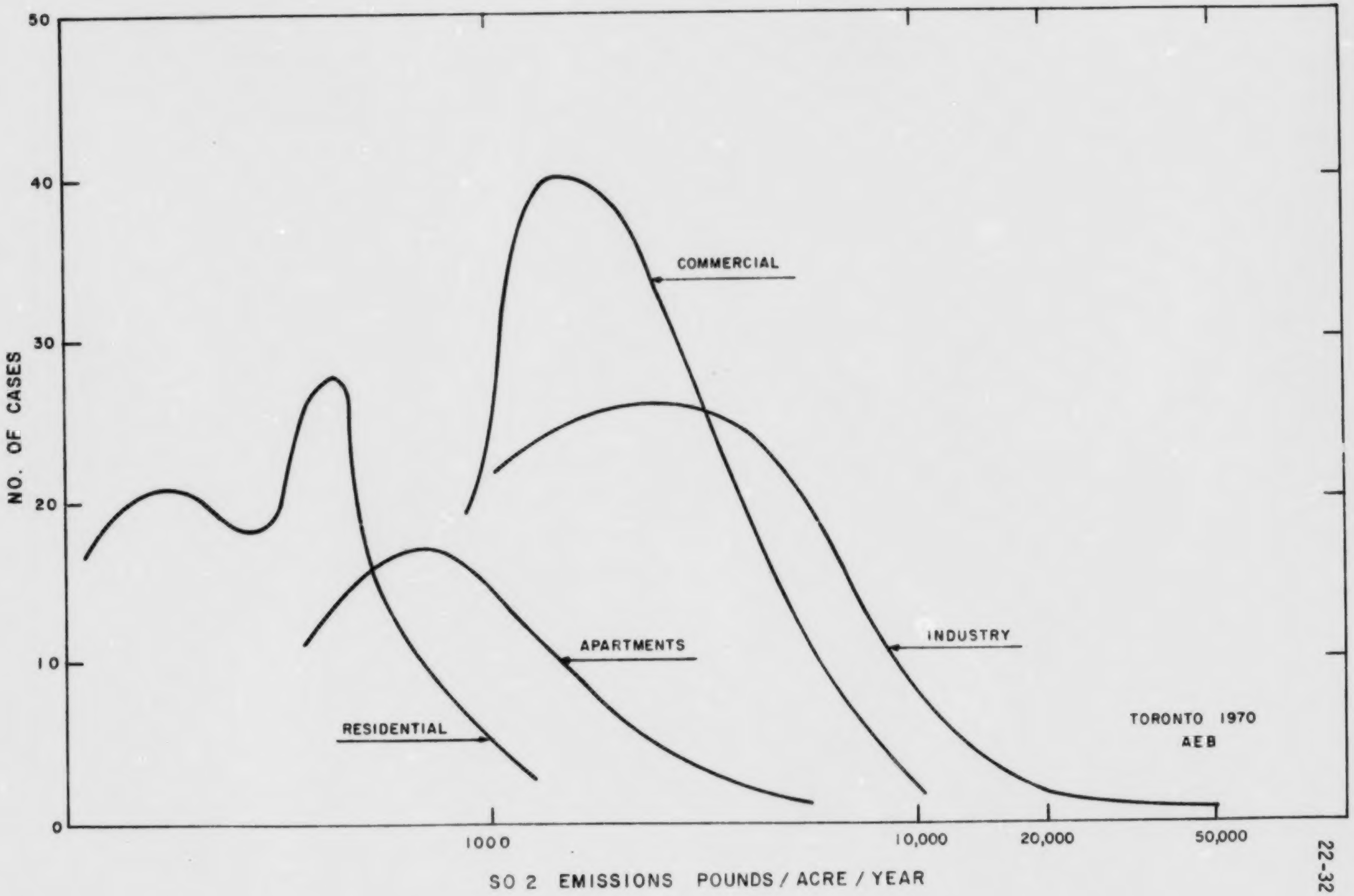


FIGURE : 8 – SULPHUR OXIDE EMISSIONS FROM COMMERCIAL BUILDINGS PER EMPLOYEE

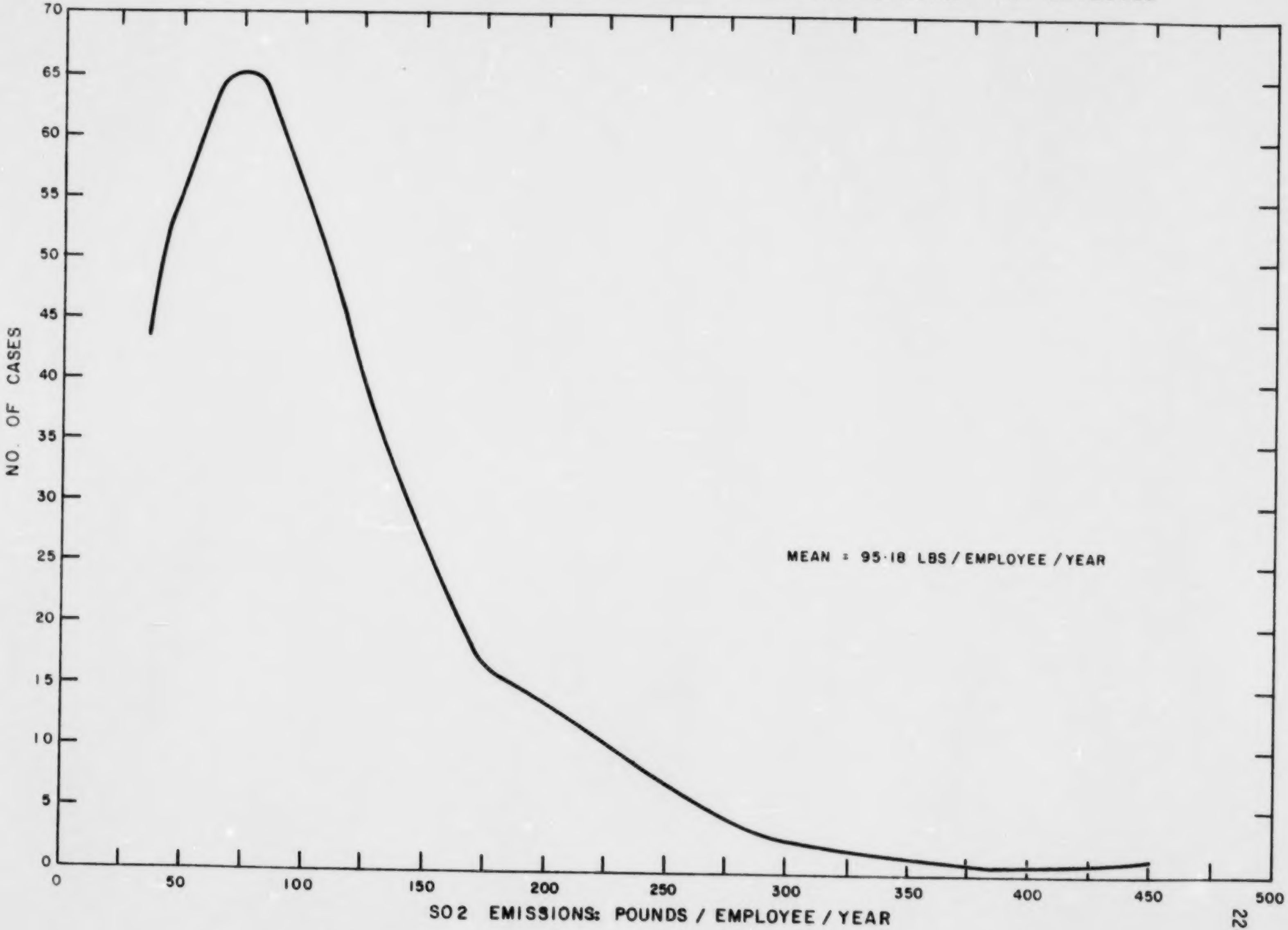
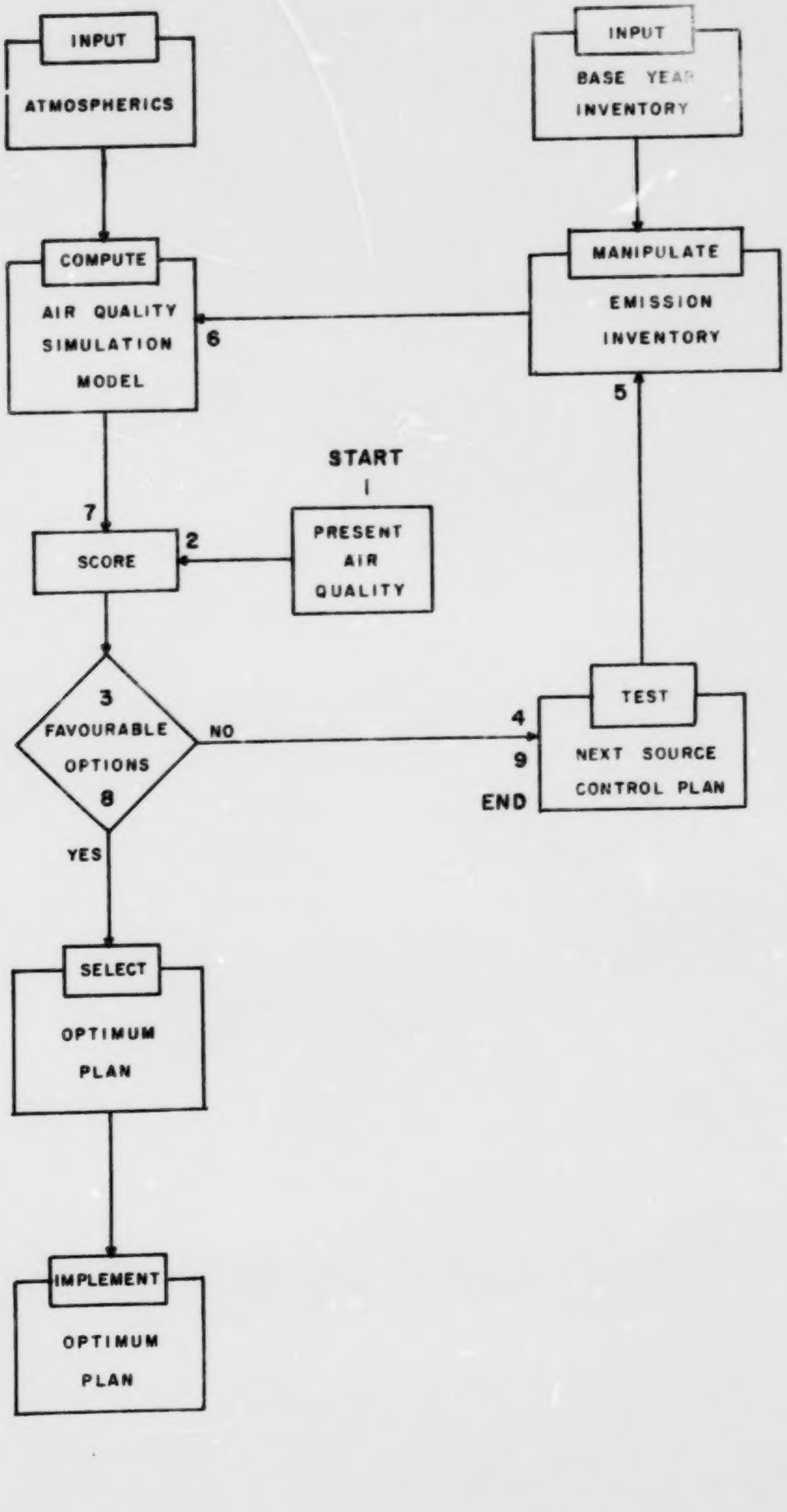


FIGURE: 9 — ATMOSPHERIC ENVIRONMENT SYSTEM


INPUT
ATMOSPHERICS
INPUT
BASE YEAR INVENTORY
COMPUTE
AIR QUALITY SIMULATION MODEL
6
MANIPULATE
EMISSION INVENTORY
5
START
1
7
2
SCORE
PRESENT AIR QUALITY
3
FAVOURABLE OPTIONS
8
NO
4
9
END
TEST
NEXT SOURCE CONTROL PLAN
YES
SELECT
OPTIMUM PLAN
IMPLEMENT
OPTIMUM PLAN

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Chapter 23

CONSIDERATIONS OF THE U. S. REGIONAL AIR POLLUTION STUDY

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

THE ST. LOUIS EXPERIENCE*

Douglas G. Fox

I. INTRODUCTION

The Environmental Protection Agency's Regional Air Pollution Study (RAPS) is now beginning in a serious way in St. Louis. I think that RAPS is what it is all about as far as air quality modelers are concerned. RAPS will be providing the most comprehensive emissions inventory ever amassed. It will be collecting the most comprehensive and best ambient air quality data ever obtained. The meteorological conditions will be better described than ever before for an urban area. All this data will be readily accessible in a set of formatted computer tapes available to the public. And the best thing of all is that everything is being done expressly for the air quality model developers. (1) The RAPS goal is to develop and validate useful air quality simulation models. I wish to underline useful because this is a key point -- the models must be useful in terms of pollution control relative to EPA's current standards. In particular, attention must be paid to existing uses of air quality simulation models and to how these models might be improved, as well as to how EPA's use of these models might be improved. In the present paper I will try to outline something of the nature of the ultimate air quality model, discuss the functions and nature of research in this field, point out some of the comparative studies which have been made in an attempt to see where model development is necessary and suggest some model validation ideas. In addition I will try to outline the RAPS program.

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*In the interests of time and the fact that Dr. Fox has not been readily available for discussions, this paper is now included without any editorial review or corrections.

Fundamentally air quality models seek to establish a connection between ambient concentrations and sources of pollution. In order to determine how good a connection is required it is first necessary to examine the standards. Table 1 is an indication of these standards. The Clean Air Act states that the concentrations indicated in Table 1 shall not be exceeded more than once in the given time period. To state what is a fundamental difficulty concisely -- the standards are extremely specific. Implicit in the specifications of the standards is a predictability that may be unreasonable. While the sources of pollution are by and large fairly regular and deterministic, as soon as the atmosphere becomes involved, a stochastic forcing function, namely, the meteorology, is important. Added degrees of unpredictability are included when the pollutant species emitted undergoes *in situ* reactions with other species already present in the ambient air. In spite of this the standards do not, at present, call for a frequency distribution or really any type of statistical description, except those implicit in the use of annual averages. For this reason it is clear that the model type required for analysis in terms of current standards must be deterministic. It must also be able to calculate changes in ambient levels at specific locations due to varying emissions. The Gaussian multiple point source model has proven most useful for applications such as these. Such models have been more useful than grid point models or trajectory models largely because of the area vs. point or subgrid scale question discussed by Dr. Roth at this meeting. A second important point in the usefulness of models relates to the information requirements of the model. Often the nature and amount of information regarding emissions and meteorology that the models require is different from that routinely available. A substantial effort must be mounted to translate the available information into the information required by the model. One can regard the air quality model as consisting of four parts, namely, the emission model, the meteorological model, diffusion and dispersion model and the transformation model. Often there is not a balanced effort between these parts and the weakest link determines the general model value. The complex models have not been developed to the point of having equal balance between the components. Hence, at present they are not as useful as the simpler models such as the Gaussian ones, although they may be a good deal superior for specific questions.

An important point regarding model validation is that one cannot develop simple and "most cost effective" models without having the complex, best possible, models available. When one begins with a simple model one is never capable of knowing the significance of what has been neglected. A further point is that being a stochastic system with many essentially unpredictable factors involved, it is really impossible to fully understand or to predict detailed behavior of pollution patterns by even the most comprehensive measurement program. Modeling offers the hope of providing a means for generating a well-behaved mean air quality region; one on which experiments can be performed and one from which a great deal of information regarding alternate planning strategies can be gleaned. A first application of complex models should be to study the question of how predictable the air quality of a region may be. The answer to a question like this would enable us to set goals for model development. It is, however, a very complex question. I do think that the Regional Air Pollution Study will provide enough data to answer some questions along this general line. We should have sufficient information to determine the relative significance of each model subroutine to the total picture.

In this context it is useful to consider briefly just what might be possible in an ultimate air quality model. Those interested in the chemistry of processes have argued for a model involving detailed transformation process simulation. Those interested in dynamics have argued that the principles of fluid dynamics must always be formally correct. A few have seen some potential consequences of the marriage between a turbulent fluid flow and the complications of chemical kinetics. In Table 2 I have tried to outline what would be involved in a full simulation of an air quality control region. Some time ago I proposed development of such a model (1), although I am not now certain that is properly a function of the Environmental Protection Agency. Nevertheless the task is one which should be considered. In order to accomplish this I would estimate about 10-man years of effort and the support of a major computing facility would be required.

Before considering the RAPS program it may be helpful to pursue the question of the usefulness of air quality models. On Table 1 are listed the EPA (and California Air Resources Board) ambient air quality standards. Notice that these represent a matrix of pollutants and time scales. The annual standards for SO_2 and TSP (Total Suspended Particulates) are well supported by our current modeling capability using the Gaussian models. The correlation coefficients between measurements and calculations generally are better than .8. Of much greater concern, however, are the 1-3 hour standards. Even for inert pollutants on the short time scales, our models do not achieve outstanding accuracy. Table 3 presents some comparisons of models with measured data for short time averages. These data are discussed more fully in Ruff and Fox. (2) I will only point out here that increasing the complexity of the model seems to increase its ability to represent the data. When chemical reactivity is included we don't really have a sufficiently detailed set of field studies to allow much comparison. Dr. Roth has referred to a study conducted by Systems Applications, Inc., to compare the three photochemical models for 6 days of Los Angeles data. These comparisons, while very interesting, are not yet conclusive.

II. The Regional Air Pollution Study

The primary components of the Regional Air Pollution Study (RAPS) are shown in Figure 1. The RAPS data base is described in more detail elsewhere (2); suffice it here to say that data will be collected and recorded with the following considerations:

(a) Data quality will be insured by a number of quality checks including a first look by the scientists involved as the data is collected and a more substantial scrutiny by the computer as it is entered into the data base.

(b) Data access will be very simply achieved through a variety of catalogue indexes.

(c) Data base will include routine analysis software, such that simple calculations such as means, contours, etc., can be performed very quickly.

The RAPS will have, for inclusion into the data base the most comprehensive emissions data set ever assembled. Specifically included within the inventory are point sources, stationary area sources, mobile area sources, mobile line sources, airports, river and railroad traffic sources, and other complex sources. An attempt is being made to provide these data on an hourly basis. Furthermore to assure that quality is high, a program of field monitoring has already begun. In addition, inventories of heat and water vapor will be prepared. These should provide information to aid in attempts to relate microvariations in meteorological and air quality patterns to land use.

The primary element of RAPS is the collection of large amounts of high quality data from the fixed station monitoring network, the RAPS special research excursions and the RAPS vertical information collection. Figure 2 is a map of St. Louis and its environs indicating the location of the 25 fixed monitoring sites. They are arranged in roughly concentric circles centered about the St. Louis arch with radii of 4, 9, 20, and 40 kilometers. Figure 3 summarizes the instrumentation at each station. At the time of this writing the details of above the surface information collection are not fixed. It is apparent that two well-instrumented helicopters will be available for limited times during the study. The helicopters are well instrumented as air quality sensors and include the capability for detecting tracers such as fluorescent particles, particle size distribution, visibility (nephelometer), NO-NO_x, O_3, CO, SO_2, CH_4, THC, temperature, dewpoint, together with the necessary recording equipment. Questions regarding the day-to-day operations of the helicopter exist. There is, however, a good deal of sentiment toward using the helicopters as a form of vertical extension of the ground network. In this mode the helicopters would fly patterns in a regular fashion around the boundaries of the region and at specified times and places within the region and perform a vertical series of measurements. These data will be available to fill out the rather complete information provided at the surface. As many of the pollutants of concern in St. Louis are reactive, the details of their concentrations as well as the meteorological environment above ground are most important. This information is essential for a full three-dimensional description of the urban atmospheric environment and to assess the behavior of air quality models. Meteorological information aloft will be accumulated from a set of 4 radiosondes released at the usual times from both inside and outside the city. In addition a program to release and track pilot balloons ("pibals") from a number of locations throughout the city will provide wind pattern information.

The final aspect of the RAPS measurement program is the expeditionary research program. Without going into any detail regarding these expeditions, I will mention three areas of research where they will be employed, namely in atmospheric transformation, meteorology, and subgrid scale studies.

There are two general areas of study in atmospheric transformations which are of interest. One is the general area of homogeneous photochemistry, the other is in the characterization of aerosol generation and growth. Some studies of plume chemistry are discussed in the subgrid scale studies subsequently. The photochemical mechanisms presently being employed in our model development require as input a good understanding of the relative initial (in early morning) concentrations of the four hydrocarbon classes, i.e., olefins, aromatics, paraffins, and aldehydes. There will be a program of routine HC breakdowns for St. Louis using samples collected from the 25 stations. Some additional bag samples will be collected and irradiated. Very extensive aerosol investigations will be performed by universities and other groups under funding from EPA. These studies are aimed at understanding the fate of SO_2 in an urban atmosphere and in particular the formation and growth of sulfates will be studied.

Meteorological special excursions are designed to do two specific tasks. The first is an extensive characterization of the St. Louis urban boundary layer. Some specific questions are; how deep is the mixing layer as a function of location and of time of day over St. Louis; what are the characteristics of urban winds, particularly during stagnation conditions; how can conditions in the city, especially regarding diffusion climatology, be modeled, given either limited information within the city or information of a synoptic nature outside the city? The second task is a study of the energetics of cities. The atmosphere in an urban area is characterized by the surface energy balance, the thermal roughness, the mechanical roughness and the external meteorological conditions. One object of the first task is to attempt to delineate the significance of each of these factors. The second task will assess the nature of the surface energy balance in the city and more specifically in diverse land use areas of the city. This will include measurement of the radiation both short (from the sun) and long (from reradiation) wave intensities in an attempt to determine the "storage" characteristics of various types of surfaces. Such characterizations will require measurement of the turbulent flux of heat, momentum, and water vapor near the surface. The effects of mechanical roughness will be studied in our meteorological wind tunnel described in detail in another paper.

A series of experiments will be designed to address the question of subgrid scale phenomena. As was stated earlier, the current models for RAPS involve solution of an appropriate set of diffusion equations. Any numerical solution of these equations must have a discretization limitation that is a physical length scale below which information is nonexistent. For most purposes about the smallest reasonable value for this scale is 1 kilometer. Since the pollution pattern over a city has much variance below this scale the model developer is faced with the problem of representing this variability to or from his model. He must develop mechanisms for incorporating point sources and line sources into the model. On the other hand, he must be prepared to justify his model results when comparisons are made to measurements at a point sensor. RAPS will study specific plumes to determine both the dispersion and the chemical reactions (SO_2 conversion and NO oxidation) they undergo. Pollutant variability and averages (over a kilometer path) will be studied at different land use sites. Long path monitors (developed under funding from EPA) operating on the principle of selective absorption of a reflected laser beam, will measure O_3, NH_3, and CO and hopefully SO_2 averages. The instruments will be tested and validated by using mobile point sensors to map the concentration distribution as a function of distance along the path. Meteorological variables will also be studied on the less than 1 kilometer basis. In particular, we will attempt to coordinate work of this sort with wind tunnel experiments.

III. Model Validation and Evaluation

Since the primary purpose of RAPS is the validation of air quality models it is well to state some of our ideas in this regard. It should be born in mind that not all air quality models are designed to do the same thing. The wide diversity in the standards (as well as in other uses) makes for a wide diversity in air quality models. Our desire in RAPS is not to limit this diversity nor, is it to proliferate the various model types, rather we wish to establish some guidelines as to the uses of models. We would hope to result with a spectrum of acceptable models with some degree of "cost effectiveness" associated with each. We are aiming to have models which are reliable and accurate and which in addition have been sufficiently well studied that probability statements can be associated with them.

Validation is a very complex and ill defined concept. I think three general approaches to the validation of a model can be considered which are: (a) comparison with data (b) sensitivity (c) physical and mathematical rigor. The most gross, and yet useful, of all these is the first. While accurate comparison with one set of data says nothing about the model's general behavior it does provide a measure of the relative accuracy of the model as well as an indication of the model's best performance. We suggest that routine comparisons be made between the various RAPS models and the concentration values measured by the RAMS. The precise nature of the comparisons is the subject of another paper which would include the specific models to be exercised in this fashion. At the very least however, as many of the models listed in Table 4 will be compared as is practical. At the very least the comparisons between calculations and measurements should include the following:

1. Correlation coefficients - Using monthly data summaries regression analysis should be performed for each of the 25 stations for 3 hr. SO_2, 1 hr. CO, 24 hr. particulate, 1 hr. oxidant and any other pollutants deemed significant. Correlation coefficients should be tabulated for each station, each month. Also longer term standards with the larger final RAPS data set should be calculated.

2. Time Series Analysis - A simple comparison of the time series of calculations and measurements at each station.

3. Other Statistical Measures - Factor analysis, χ^2 tests, etc., on the pollutants of interest.

4. Analyzing the time series - Use of orthogonal functions with decomposition to separate random and nonrandomness in the signals.

Sensitivity analysis has always provided the modeler with a good measure of his model's abilities. A successful model will have sensitivities which mirror the system being simulated. A recent study (3) of Gaussian multiple point source models has shown that these models are highly sensitive to wind direction, the size of area sources and the dispersion coefficients selected. Results of other work currently underway to study the sensitivity of the more complex models suggest the need for good meteorological wind fields and mixing depths over the city, initial conditions, i.e., the initial amount of pollutants present are also important. The RAPS will investigate the sensitivity of all of the models in Table 4 to both external parameters and internal parameters. For the Gaussian based models the external parameters are -- wind direction, area and point source strength, area source height and receptor location. It is straight forward to study the sensitivity of the model to variations of such parameters. Internal model parameters are the mixing depth and σ_z as a function of distance, the manner in which plume rise is calculated and how the sources are treated. Since there are a great many different ways of treating each of these some thought must go into just how much fiddling with the models will be done. The complex models will receive a good deal more consideration. In an initial study we are considering the sensitivity of such models to the windfield. Is it necessary to have a fully three dimensional fine resolution windfield provided each hour? How much can one back off this requirement? To what degree must the mixing depth be specified? Generally the turbulent transport of pollutant is accomplished in such models with horizontal and vertical eddy diffusivities. How much sophistication is necessary in the specification/calculation of these terms? There are fundamental questions relating to how one extrapolates from a point source to the grid average value and in turn how one interpolates to a point receptor from the grid averages. All of these aspects must be studied in a detailed program currently being developed.

The third principle namely of "good" science, is common sense. Given the choice between two modeling methodologies, in the absence of other determining factors, that model which pays closest attention to proper mathematics and physics should be chosen. An example might be the presence of numerical diffusion, so called artificial diffusion, prevalent in non-centered finite difference schemes. The effect of such diffusion is to reduce the intensity of the signal, i.e., diffuse the pollutant. Indeed, successful schemes for solving the equations have taken advantage of the numerical diffusion by reducing the magnitude of the physical diffusion coefficient. While this can work it is not always successful since, for example, if one wanted to calculate dispersion of a pollutant under very stable conditions the numerical diffusion would be unacceptably large and quickly swamp out the signal. There should be a progression toward better and better models. It should always be possible to improve models and thus models which are capable of handling greater complexity and improvement should be preferred over other models. It is impossible to be very certain about how well or how "cost effective" a simple model is without having a much more complex and realistic process simulation model available against which to test the simple model.

Finally, I would like to suggest a final form for the RAPS model and for the validation study. Consider the model table shown in Table 5. In this table an attempt has been made to segment the various degrees of complexity involved in each component of the total air quality simulation model. The table is self explanatory. We would hope to evolve a set of computer programs to perform the work in each module. These programs might be written such that they could be patched together to form a complete model. Then one could look at the effect of each particular level on the entire model. Hopefully what would evolve is something like shown pictorially in Figure 4. According to the desired use one could choose the "best" model for his purposes. Conceivably the measure of goodness on the ordinate would vary from application to application while the abscissa could represent a cost of achievement. Obviously a good deal more work is required to implement these ideas.

IV. Summary

It is premature to have any conclusions regarding the RAPS. I wish only to leave you with the concept that the study will be a dynamic one. Nothing is so fixed as to not be changeable as evidence is accumulated in one direction or another. There will always be room for modelers to suggest experiments and procedures. We hope that the RAPS data will be sufficiently accessible for the modeling community to make use of it and on that basis suggest what we should do to improve and update the study.

ACKNOWLEDGMENT

I wish to acknowledge several discussion with the Model Development Branch and in particular with John Clarke in which most of the ideas in Section III were formulated.

Figures 1 and 2 were graciously provided by Dr. Shepard Burton and

Mr. James Reagan.

I would like to acknowledge assistance gained through many discussions on the RAPS programs with Drs. McElroy, Stevens and Ruff, and especially Dr. F. Pooler, Research Coordinator.

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Table 1

EPA STANDARDS   P = Primary,   S = Secondary   C = CARB

Time Average \ Pollutant	SO_2 (ppm)	TSP ($\mu g/m^3$)	NO_2 (ppm)	CO (ppm)	O_x (ppm)	NMHC (ppm)	SO_4 =
Annual	.03 (P) .02 (S)	75 (P) 60 (S) 60 (C)	.05 (P) (S)				
24 hour	.14 (P) .10 (S) .04 (C)	260 (P) 150 (S) 100 (C)					
12 hour				10 (C)			
8 hour				9 (P) (S)			
3 hour	.5 (S)					.24 (P) (S) 6am - 9am	
1 hour	.5 (C)		.25 (C)	35. (P) (S) 40 (C)	.08 (P) (S) .10 (C)		

Table 2

Emissions Inventory

Source Type	Spacial Resolution	Pollutants	Temporal Resolution
Point	within 10 meters	SO_2, NO_x, CO, RHC, Particulates	Minute perhaps, second
Area	1 km or less	SO_2, NO_x, CO, RHC, Particulates	1 Hour
Line	> 1 km located within 10 meters	CO, SO_2, Particulates	5 Minutes
Special	as necessary	as necessary	as necessary

Atmospheric Environment

I. Full three dimensional solution of the equations of motion for a turbulent atmosphere over an urban area

- lateral boundary conditions specified by large scale meteorological model
- surface boundary conditions specified by detailed energy balance
- resolution of the order of 1 km and 10 minutes
- turbulence model to parameterize transport to smaller scales.

II. Subgrid scale flow field

- lateral boundary conditions from I above
- detailed turbulence model capable of generating a reasonable flow required for the subgrid scale
- extremely fine time and space resolution

Transformation and Removal

Process simulation of gas phase chemical reactions

Process simulation of heterogeneous chemical reactions

Simulation of the gas phase -- heterogeneous interactions

Detailed simulation of aerosol growth both physical and chemical

Nesting process simulations into both the subgrid scale and urban scale flow field models

Interactions between urban atmospheric chemistry and natural meteorological processes.

- cloud condensation nuclei (rain out)
- removal of pollutants by surface scavenging

Table 3

Correlation Coefficient Between Calculation and Measured Data from St. Louis

Sta. #	Gaussian Plumes[3]	Simple Box Model[4]	Grid Point Model[5]	Comments
3	.20	.20	.33	in sources
4	.29	.37	.19	in sources
10	.24	.05	.23	in sources
12	.46	.53	.65	in sources
15	.45	.54	.48	
17	.39	.41	.44	
23	.25	.60	.49	
28	.36	.53	.64	
33	.40	.57	.59	
36	.44	.49	.62	
Overall	.35	.39	.53	

Table 4

URBAN MODELS AVAILABLE

		Require Meteorological Field		
POLLUTANT CATEGORY	SOLUTION MODELS	TRAJECTORY MODELS	GRID TYPE MODELS	OTHER
Nonreactive Point & Area Sources	CDM SCIM		IBM	USM
Decay Point & Area Sources	SCIM	Development		
Reaction Mech. Point & Area Sources	Development			
Nonreactive Mobile Sources	APRAC	GRC PES	SAI	
Reaction Mech. Mobile Sources		GRC PES	SAI	
Reaction Mech. All Sources			Development	
Removal Processes	Development		Development	

Table 5

EMISSIONS	METEOROLOGY	DIFFUSION AND DISPERSION	TRANSFORMATION AND REMOVAL
LAND USE ANALYSIS 1	RURAL WIND + SOUNDING (AIRPORT) 1	GAUSSIAN PLUME (PUFF) MODELS 1	LINEAR EXPONENTIAL DECAY 1
MAJOR SOURCES ONLY 2	MEAN SURFACE WIND & SOUNDING (NETWORK) 2	COLUMN TRAJECTORY MODEL 2	PARAMETERIZED MECHANISM 2
NEDS INFORMATION 3	SURFACE WIND FIELD & TEMPERATURE STRUCTURE 3	BOX WELL MIXED 3	PROCESS DESCRIPTION 3
LIMITED SPECIAL STUDIES 4	THREE-DIMENSIONAL WIND FIELD TEMP. & HUMIDITY 4	THREE DIMENS. GRID MODEL 4	DEPOSITION VELOCITY 4
FULL RAPS EMISSION INVENTORY 5	PREDICTED WIND & OTHER FIELDS 5	FULL GRID + TURBULENCE MIXING PROC. 5	FULL PRECIP. REMOVAL 5

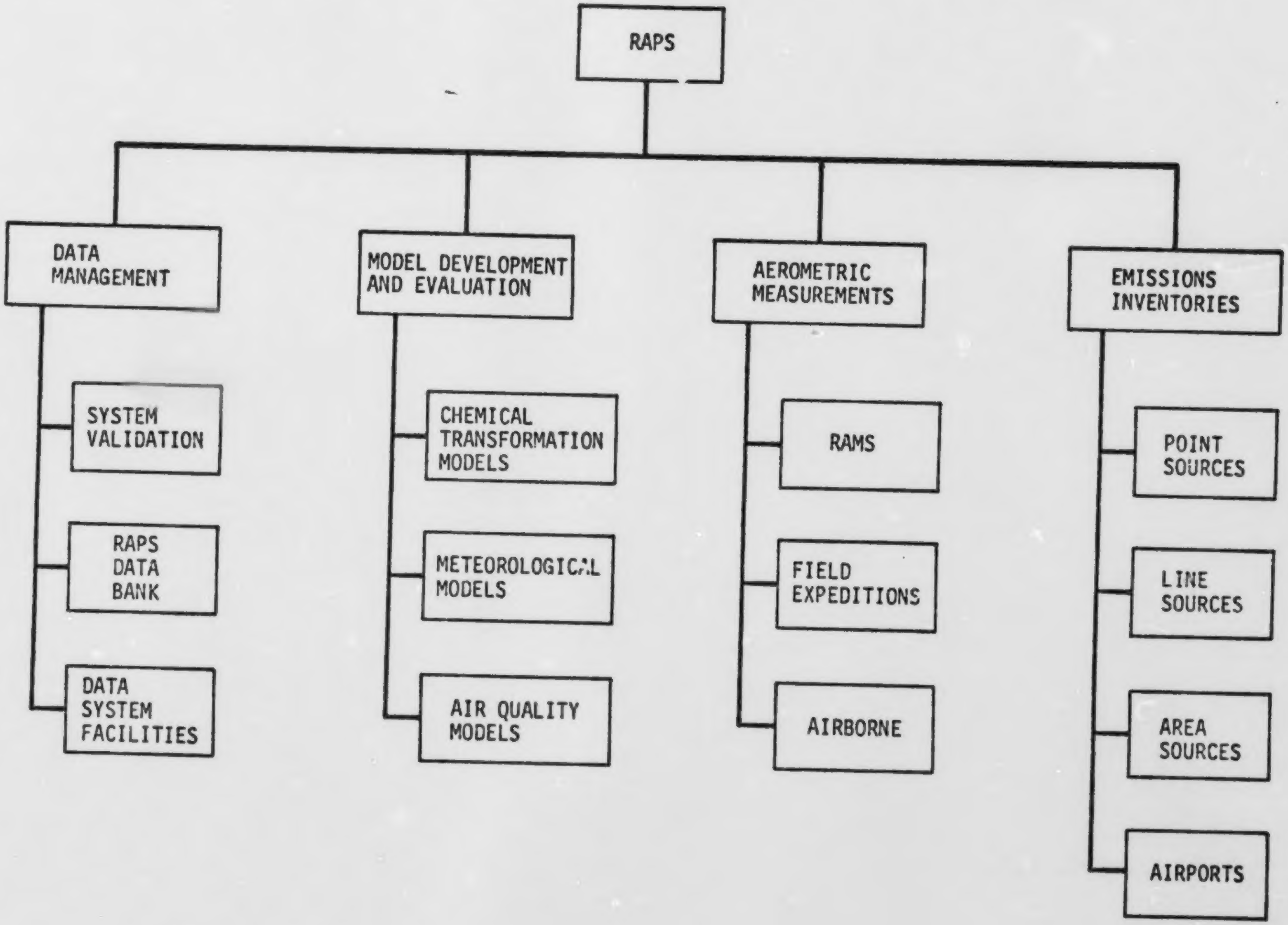
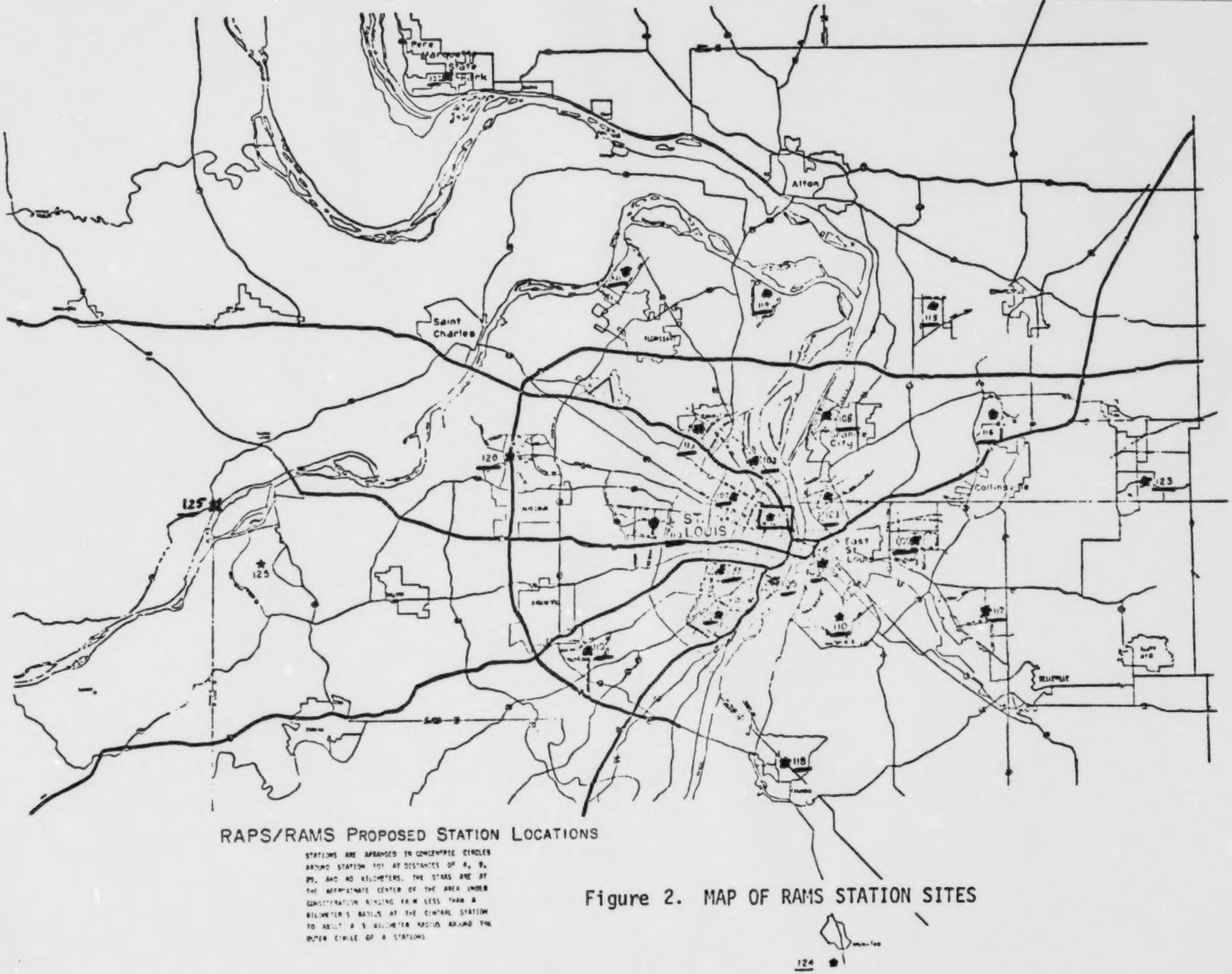

RAPS
DATA MANAGEMENT
SYSTEM VALIDATION
RAPS DATA BANK
DATA SYSTEM FACILITIES
MODEL DEVELOPMENT AND EVALUATION
CHEMICAL TRANSFORMATION MODELS
METEOROLOGICAL MODELS
AIR QUALITY MODELS
AEROMETRIC MEASUREMENTS
RAMS
FIELD EXPEDITIONS
AIRBORNE
EMISSIONS INVENTORIES
POINT SOURCES
LINE SOURCES
AREA SOURCES
AIRPORTS

Figure 1. PRINCIPAL ELEMENTS OF REGIONAL AIR POLLUTION STUDY (RAPS)


Pere Marquette State Park
Alton
Saint Charles
St. Louis
East St. Louis
Granite City
Collinsville
Belleville
101
103
106
110
112
113
115
116
117
118
119
120
122
123
124
125

RAPS/RAMS PROPOSED STATION LOCATIONS

STATIONS ARE ARRANGED IN CONCENTRIC CIRCLES AROUND STATION 101 AT DISTANCES OF 4, 9, 20, AND 40 KILOMETERS. THE STARS ARE AT THE APPROXIMATE CENTER OF THE AREA UNDER CONSIDERATION RANGING FROM LESS THAN A KILOMETER'S RADIUS AT THE CENTRAL STATION TO ABOUT A 5 KILOMETER RADIUS AROUND THE OUTER CIRCLE OF 4 STATIONS.

Figure 2. MAP OF RAMS STATION SITES

RAMS Instrumentation

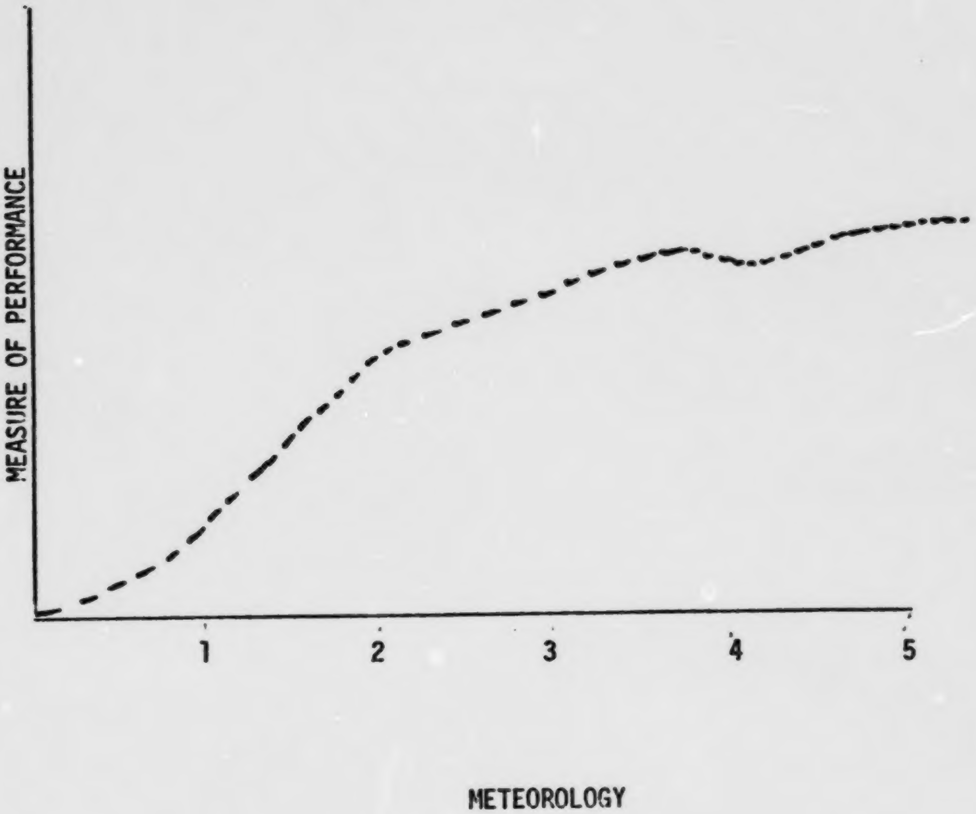
Network

25 stations
Automatic operation, PDP - 11/40 central computer
Telemetered digital information plus data
acquisition each station
1 minute interrogation
Display by CRT and printer/plotter
Mag tape storage

Station Instrumentation (all stations unless specified)

Ozone
NO, NO_2, NO_x
CO, CH_4, NMHC
Total Sulfur (12 sta)
H_2S, SO_2, TS (13 sta)
Gas Bag Samplers
Particulates: Hi-vol filters (5 sta. Dichotamous sampler with 2μ separation (12 sta)
Nephelometer
Wind, speed and direction
Ambient temperature
Differential temperature (12 sta, 30-meters)
Dew Point
Pressure (7 sta)
Solar radiation:
4 stations: three spectral pyranometers
one direct pyreheliometer
one long wave pyrogeometer
2 stations: two spectral pyranometers
Turbulence (5 sta, u, v, w, local recording only)

Figure 3



SO_2 SECONDARY 3 hr. STANDARD

E4 -- M3 -- D4 -- T1

SULFATE MODEL

E5 -- M5 -- D5 -- T35

Figure 4

Chapter 24

A COMMON DATA BASE FOR AIR QUALITY MODELING

by

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U. S. Environmental Protection Agency

5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

I. Background

In workshop sessions of the Fourth Meeting of the Expert Panel on Air Pollution Modeling, several references were made to shared data and models. During the session on the Role of Regional Air Pollution Studies in Model Development, Drs. L. E. Olsson (Sweden) and D. G. Fox (U.S.A.) discussed the desirability of forming a common data bank from the United States RAPS project. The objective of this endeavor would be to provide a data bank for test and comparison of air quality models.

The type of data bank desired would reside on a universally compatible magnetic tape and consist of a test data set of about 30 days, consisting of one-hour averages for wind speed and direction, atmospheric stability, pollutant concentrations, and emission inventory estimates. It was further suggested that the RAPS data would be the best available for this purpose. Part of the RAPS data management objective is to avail such a tape to the general public. A tape containing data as described above should be available within the next year.

In his introductory remarks at the Fourth Meeting, Professor W. Klug (West Germany) outlined broader common data requirements than discussed in the previous paragraph. The availability of data spanning several years was emphasized. It is noteworthy that the data requirements for modeling the atmospheric chemical transformations were not mentioned. This of course adds greater complexity to the data base. Furthermore, data from RAPS is just a start in the formation of a common data base. Other data will be needed to insure that model validations are not restricted to St. Louis.

The Environmental Protection Agency (U.S.A.) has established data bases which are useful in model development and application. The National Emissions Data System (NEDS) and the Storage and Retrieval of Aerometric Data (SAROAD) provide a comprehensive, nationwide source of emissions, air quality, and meteorological data. Though these data are useful in validating simple air quality models, they are not comprehensive enough to support a state-of-the-art model development program. This was well recognized and led to the formulation of the RAPS program.

So far, discussion has centered around traditional concepts of data which imply measurements reduced from meteorological and chemical sensors. The concept of data can, and perhaps should, be broadened even to the point of including source statements for the models themselves. There are sound arguments for inclusion of details of the models in the data bank. Without these technical details on models, (1) comparisons are reduced to those between black boxes, (2) technology improvements are not shared in a timely manner, and (3) redundancy in model development effort abounds as it has in the past with the Gaussian formulation.

II. Implementation

The establishment of a common data base at any realistic level is well within the reach of today's computer technology. Before implementation, the modeling community must first agree on the type and quantity of data needed. Since one modeler's requirements almost always differ from another's, the formation of an interdisciplinary committee is indicated. This committee would define objectives, establish content, and oversee dissemination. The important point is that the common data bank must satisfy the general needs of the modeling community as a whole.

Techniques for data distribution will vary as the requirements vary. If the common data base were as simple as the one Olsson and Fox discussed, then a magnetic tape distribution mechanism would be appropriate. This type of distribution can be handled within the framework of the National Technical Information Service (U. S. Dept. of Commerce). A single tape can easily contain the quantities of data required.

Establishment of a common data bank for the quantities of data suggested by Klug is not so straight-forward. The RAPS data base in a period of two years will accumulate over one billion words. When dealing with quantities of data this large, one looks for alternatives to tape transfer for a number of reasons. No longer is it a matter of representing the data base on one tape; it is now contained on over one hundred tapes. Of the one billion words, most scientists are probably interested in only a small percentage of the data. However, this small percentage may be spread out over several tapes. Furthermore, it may be necessary to interact with the data base so that one is constantly requesting small quantities of data in an iterative analysis.

In the design of the RAPS data management system, the needs of all the RAPS scientists have been incorporated into the plan. The data base will reside on a Univac 1110 computer system, In addition to standard compilers for Fortran V and Cobol, the system support includes the data management language System 2000, developed by MRI Systems Corporation of Austin, Texas. This language facilitates file organization, data loading, access, and retrieval software. Some of the most frequently used data will be accessable on demand from an interactive terminal. The remainder will be archived in the tape library but will be retrievable on-line in minutes (the time it takes to mount and scan the appropriate tapes). A set of "canned" statistical and plotting programs will be readily available for a first-look analysis of the data. For more complicated analyses, special formatting software will be provided to link the data base to any computer analysis program.

The above system will be a great asset to EPA scientists and certain EPA contractors. However, it falls short of availing the RAPS data to the general scientific community. The Univac 1110 system was never intended to fulfill this need. Ruling out this possibility, the question remains on how best to fulfill the common data bank requirement.

One extreme in disseminating a large data base is to copy tapes for every user installation. For the number of tapes involved, this is a cumbersome, wasteful process. From a systems analyst's point of view, it is a poor choice because of a multiple duplication of computer storage and processing. Each investigator must separately install and debug the data base on his own computer (a tedious process). Some investigators may not even have the facility to do this. This technique of dissemination, for large quantities of data, is not one that lends itself well to the common data base concept.

The opposite extreme in implementing a large common data base is the large computer and multiple remote terminal approach. This is the same concept being used within EPA for the RAPS data base. The basic differences are that only a small portion of the modeling community has access to it and that the remote terminals are not spread out over a large geographical area. These are not technological problems. The point is that, with present technology, a powerful enough computer system can be assembled to satisfy the data base needs of the modeling community. The resulting base would include all the RAPS data, of course, but also data from other relevant research projects. The overriding issue here is the cost/benefit figures. If the benefits justify the cost, can a source of funding be found? The previously suggested committee must answer such questions.

For the near future, the super computer approach does not represent a practical solution. An alternate means of implementation is to install the data base on just a few computers with common software. As related to the RAPS data base, the common software would include the Fortran V and System 2000 compilers and the majority of the installation, retrieval, and analysis programs written in those languages. Furthermore, each computer system must support some of the same software specific peripherals such as Calcomp plotters and remote batch and interactive terminals. This is a practical approach which would not require excessive costs.

In addition to common software and peripheral support, the chosen computers must be available to the entire modeling community and capable of supporting this additional load. Computers that can satisfy these criteria exist today in sufficient quantity.

III. Summary

This paper has only briefly touched on the complications associated with a common data bank. In the next year or two, the RAPS data dissemination should be accomplished as suggested by Olsson and Fox. Recommendations should be drafted for a set of data requirements on this smaller scale first. This set should meet the common needs of the modeling community.

As a second step, it is recommended that an interdisciplinary study be made on the detailed data requirements of the community. The data should encompass RAPS and any other relevant field studies. This study will serve as a foundation in the development of a common data base mechanism.

Chapter 25

VALIDATION OF URBAN AIR POLLUTION DISPERSION MODELS

by

L. E. Olsson and S. Ring
Swedish Meteorological and Hydrological Institute

5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

VALIDATION OF URBAN AIR POLLUTION DISPERSION MODELS

Lars E Olsson and Sture Ring
The Swedish Meteorological and Hydrological Institute

As we attempt to simulate the dispersion of air pollution in an urban area with a numerical model we are, in an "engineering sense", trying to find the mathematical function that best transfers source strength data into environmental air quality. What model approach we choose is primarily dependent on the purpose with the simulation and the degree of physical complexities encountered in the area. A good understanding of the dispersion process is necessary if the model formulation is to be physically sound. Several papers have been published and also discussed at these NATO/CCMS meetings dealing with different kinds of models and their ability to "reproduce" measured air quality, eg Fortak (1969), Gifford (1973), Bringfelt et al (1974), Grönskei (1973), Egan (1971). A simplified flowchart illustrating the development of a dispersion model is presented in Figure 1.

The basic input parameters to any meteorological dispersion model are, besides source strength fields, wind speed and direction, some dispersion parameter normally related to atmospheric stability and the mixing height. Different types of models might be more or less sensitive to errors in some of these input parameters normally depending on desired time and space resolution. The importance of analysis of the model sensibility in connection with model validation has been discussed eg by Johnson (1972) and in the report by Koch et al (1971) presented by Calder at this meeting.

For validation purpose the modeller is normally given a set of simultaneous source, meteorological and air quality data. Depending on how well the calculated air pollution concentrations agree with those measured the model is said to be "good or bad". There is however no simple measure that can be used to judge the "goodness" of the model. Some of the most common ways to present model validation analyses are discussed in this paper.

In evaluating the validation results one has to consider the meteorology of the validation period. Especially if the period is short it might be necessary to adjust the results to climatological averages and extremes eg by filtering out certain portions of the data. Any validation test should include a thorough analysis of the data used especially with regard to data representability and quality. Furthermore it is important to consider the expected use of the model eg in connection with different types of air quality standards.

Time serie comparison

By simply making a time serie plot of the measured air quality and that calculated at a receptor point or averaged over some area it is possible to obtain a qualitative measure of the model goodness. In judging the comparison it is necessary to consider the spacial representability as well as the temporal resolutions in measured and calculated concentrations respectively. This type of presentation is especially useful in analysis of a model's capability to reproduce diurnal or other temporal cycles.

Regression analyses

A scatter diagram and a regression line with suitable statistical measures give at least a semi-quantitative evaluation of the model goodness. This analysis technique can be used on different time- and space-averages. An example of this type of analysis used in the evaluation of a gaussian type urban air pollution dispersion model, Bringfelt et al (1973) is given in Figure 2. The model treats area and point sources separately and has been applied to three different urban areas where the ratio between area source and point source SO_2 emissions are quite different. In Stockholm 65%, in Gothenburg 39% and in Malmö only 11% of the emitted SO_2 comes from area sources, mainly space heating.

It is obvious from this type of analyses that the model has a tendency to over-estimate contributions from area sources and probably under estimate point source contributions.

The model calculates concentrations in the centre of a grid 500 x 500 m^2 (for Stockholm and Malmö) or 1 x 1 km^2 and those are compared with measured concentrations at some location within the grid area. In Figure 3 are measured concentrations at locations close to each other plotted in a scatter diagram giving a qualitative picture of the variance to be expected due to inaccuracies and lack of area representativities in the measurements.

Correlation

If a model perfectly reproduces the actual temporal air quality variations the correlation coefficient would be 1.0. As discussed above there are problems in getting a representative and accurate measure of the air quality. Furthermore the relative errors in the measurements are dependent on the magnitude of the concentrations measured. In comparing series of measured SO_2-concentrations at locations close to each other it is possible to get an estimate of what would be a reasonable degree of correlation. Based on several months of such comparisons of 24-hour average concentrations it is suggested that a correlation above 0.4 would be satisfactory in cases when the 500 x 500 m^2 grid is used. An average correlation between pairs of measurement series was 0.65 if the SO_2-concentration exceeded 4 pphm.

Error range

Besides comparing different averages, variances and standard deviations it is sometimes useful to look at what has been termed the "error range" defined as the "root mean square error" divided by the mean measured concentration, Marsh and Withers (1969). In analyzing several months of pairs of 24-hour measurement series it is suggested that an error range less than 0.5 would be satisfactory when the 500 x 500 m^2 grid is used. An average error range of 0.4 was calculated assuming that one series represented the true air quality.

The values given on correlation coefficient and error range are suggested based on analyses of the data used in the validation program for a model applied to three cities in Sweden and are only used to exemplify this discussion. The degree of correlation and the maximum acceptable error range is dependent on several factors related to specifies of the model area and application.

Frequency distribution

For the model applications the frequency distribution of air pollution concentrations is of interest and in several countries the standards are directly related to this, eg in Sweden where the 1/2-hour SO_2-concentration should not exceed 25 pphm more than 1% of the time in any 30 day period. Larsen (1968) has shown that the logs of the concentrations in an urban area are normally distributed eg there will be a straight line on a log-normal plotting paper. By plotting the frequency distribution for different wind direction sectors it is possible to analyze the model response selectively.

An example of this type of validation presentation is presented in Figure 4.

Spacial distribution

Validation analyses with an urban area air pollution dispersion model capable of calculating concentration fields in a grid should include a study of the spacial distributions of calculated and measured concentrations. Such a study might explain why any one "receptor-station" fails to validate. In Figure 5 the "next to max" calculated 24-hour SO_2-concentration field for one month is presented. The underlined numbers are the next highest measured 24-hour SO_2-concentrations for the same month.

As can be seen in Figure 5 there seem to be poor agreement in some points eg the 7.6 vs 16.2 in the SE corner of the field. This error appears in several analyses and can be explained by the topography in the area. If the field, due to a slight change in wind direction is moved 2 gridpoints west, eg 7.6 vs 6.8, there would appear to be almost perfect agreement. Similarily minor adjustments of the model had to be made in other parts of the model area eg in the NW portion.

We have tried to show that the validation proceedure of an urban air pollution dispersion model by no means is a straight forward process. On the contrary we have to use all our knowledge and skill in trying to judge the "goodness of a model". The planned use of the model, the meteorology and physical characteristics of the model area as well as the quality of the data has to be foremost in our minds as we attempt to make this judgement.

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Marsh. K.J., and W.R. Withers (1969): An experimental Study of the Dispersion of the Emissions from Chimneys in Reading-III: The Investigation of Dispersion Calculations. Atm. Env. 3, pp. 281-302

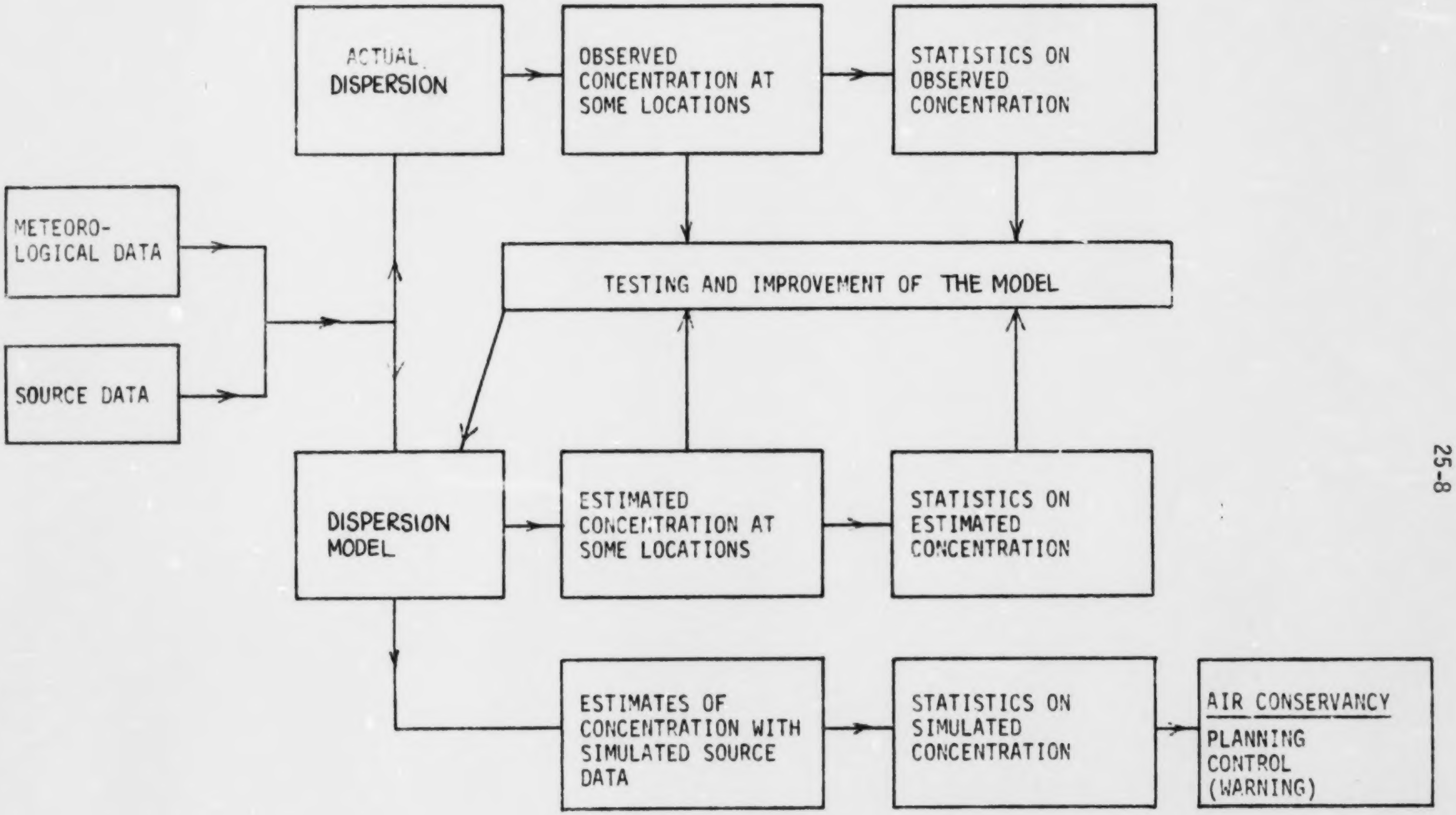
ACTUAL DISPERSION
OBSERVED CONCENTRATION AT SOME LOCATIONS
STATISTICS ON OBSERVED CONCENTRATION
METEORO-LOGICAL DATA
SOURCE DATA
TESTING AND IMPROVEMENT OF THE MODEL
DISPERSION MODEL
ESTIMATED CONCENTRATION AT SOME LOCATIONS
STATISTICS ON ESTIMATED CONCENTRATION
ESTIMATES OF CONCENTRATION WITH SIMULATED SOURCE DATA
STATISTICS ON SIMULATED CONCENTRATION
AIR CONSERVANCY
PLANNING
CONTROL
(WARNING)

Figure 1. Flowchart for the development and application of an air pollution dispersion model.

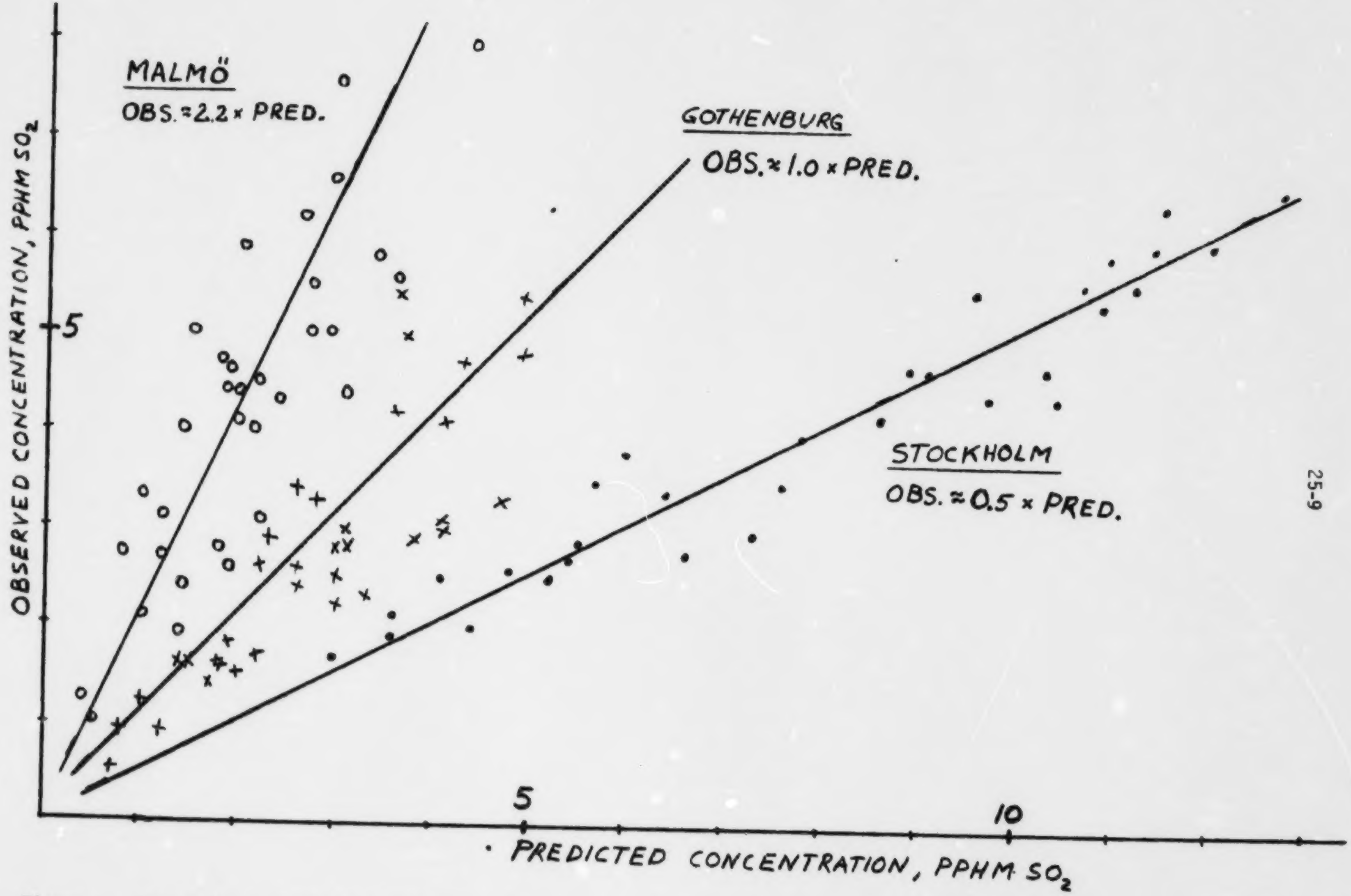

Figure 2. Regression analysis of monthly mean SO_2-concentrations for several stations in Stockholm, Gothenburg and Malmö, Sweden.

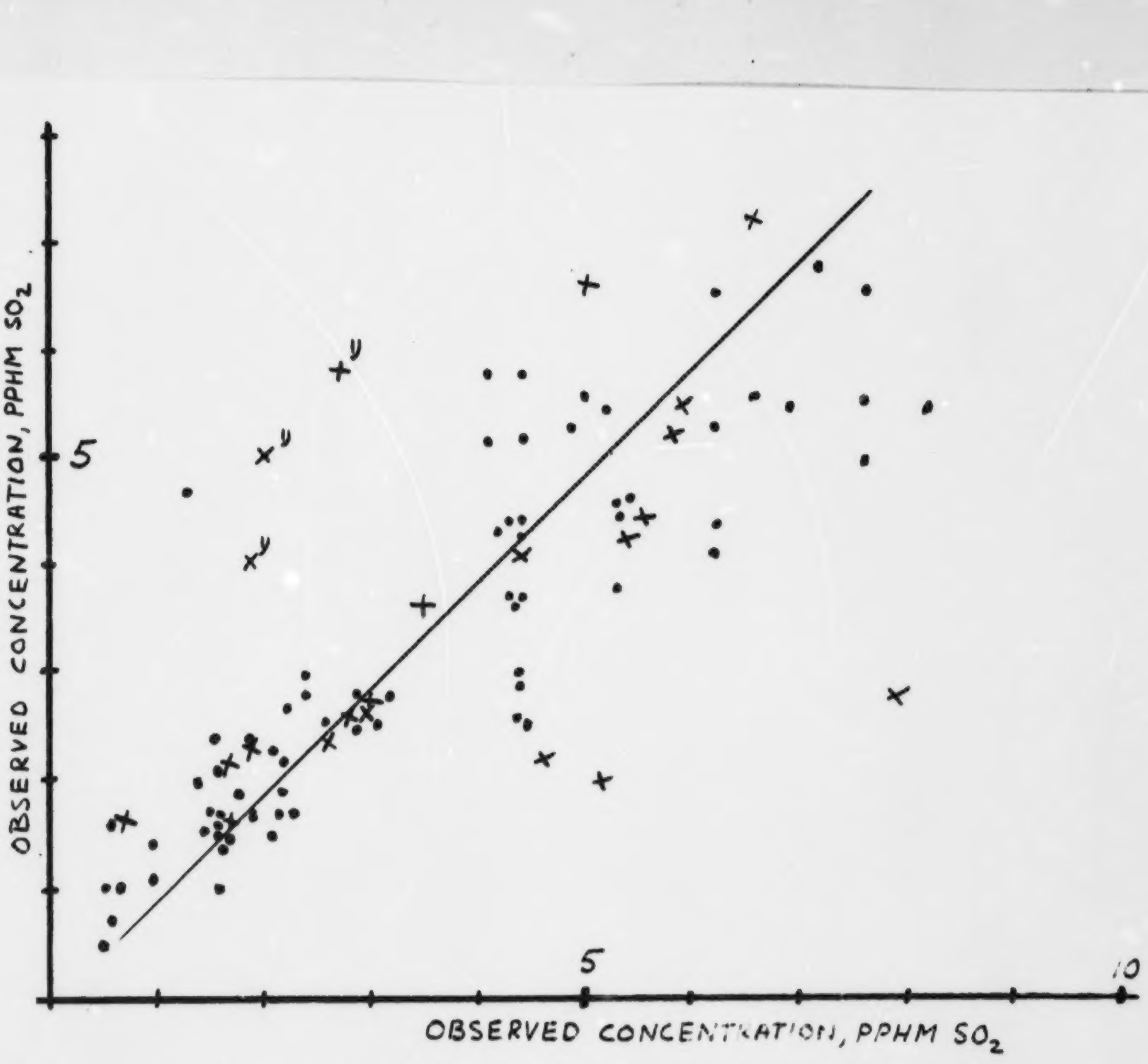

Figure 3. Regression analysis of monthly mean SO_2-concentrations measured at stations in Stockholm, Gothenburg and Malmö, Sweden. X: distance between the two stations less than 500 m. ●: distance less than 2300 m. 1) Different measurement techniques were used at the same station.

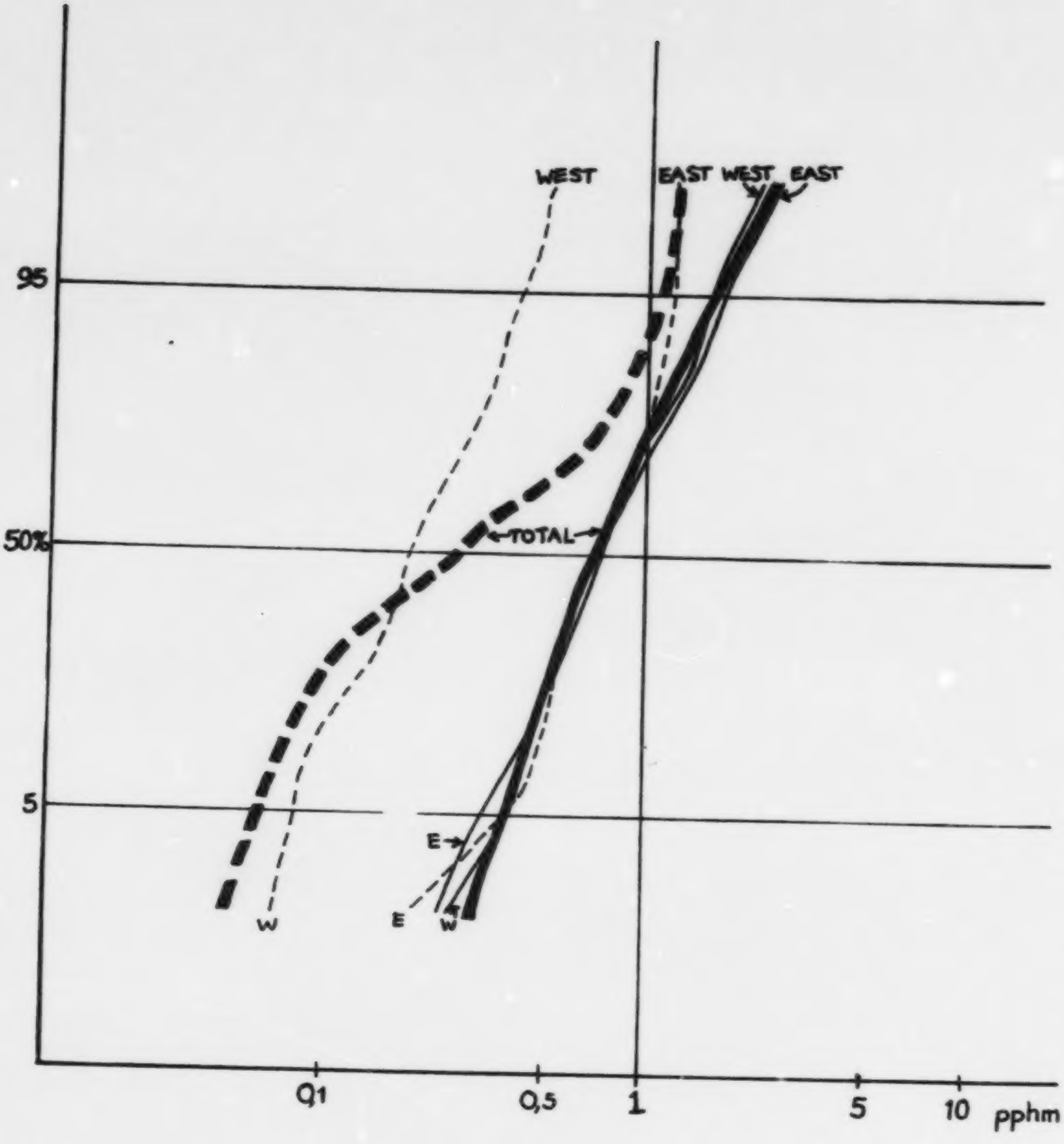

Figure 4. Frequency distributions of measured (—) and predicted (---) one-hour SO_2-concentrations in pphm for one month at one station-receptor point.

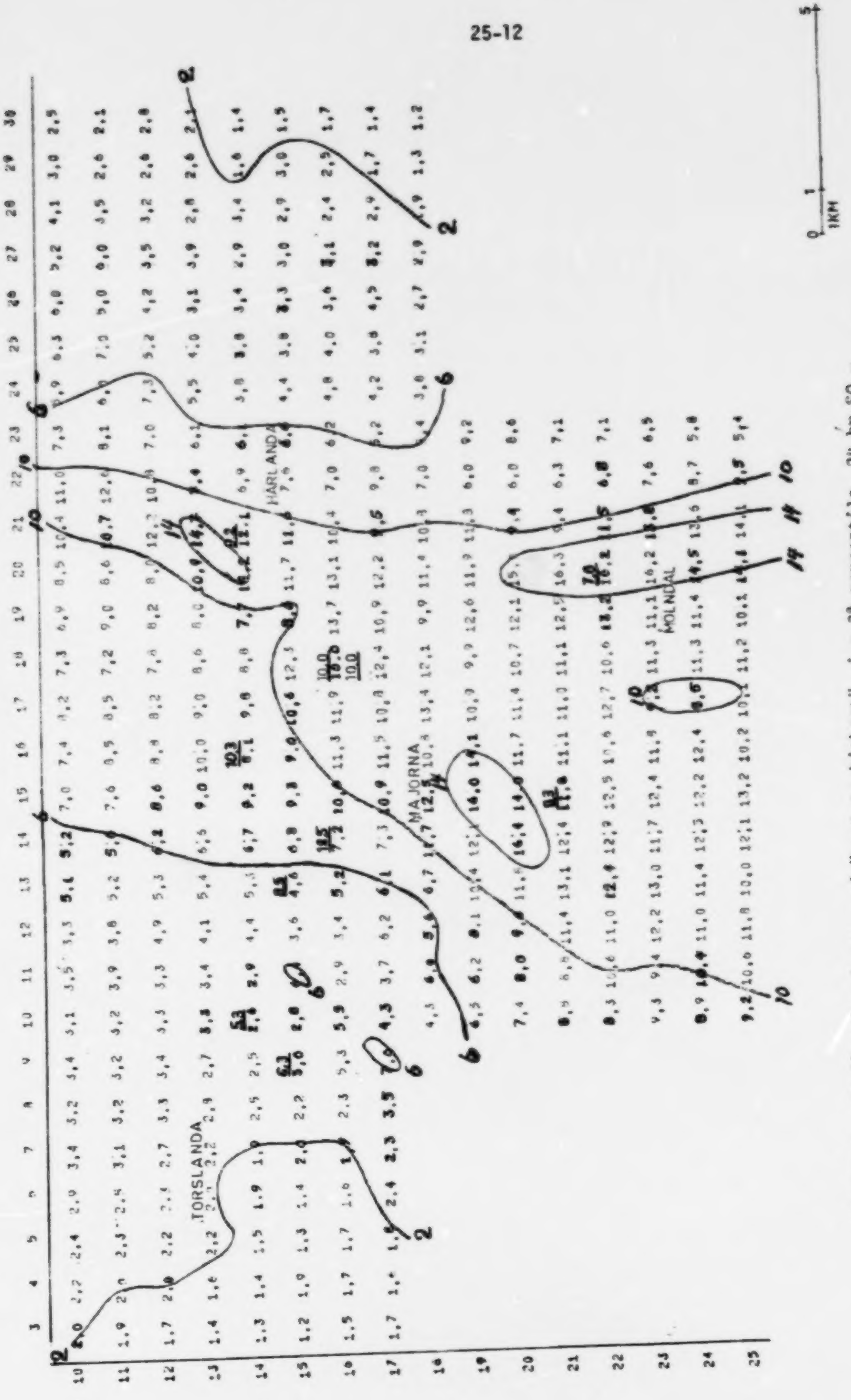
TORSLANDA
MAJORNA
HARLANDA
MOLNDAL
0
1
5
1KM

Figure 5. Predicted and measured "next to highest", i e 3% percentile, 24 hr SO_2-concentration in a month for Gothenburg, Sweden.

Chapter 26

VALIDITY AND SENSITIVITY ANALYSIS OF THE GAUSSIAN PLUME MULTIPLE-SOURCE URBAN DIFFUSION MODEL

by

Robert C. Koch and Scott D. Thayer
Geomet, Incorporated, Rockville, Md., U.S.A.
(Remarks presented by K. L. Calder)

5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

Mr. Calder said that as time was so limited he would not even give the talk he had prepared on this topic, and which was based on two short papers by Messrs. Robert C. Koch and Scott D. Thayer of Geomet, Incorporated; Rockville, Md., U.S.A. These papers would be reproduced in the Proceedings of the 5th Meeting. They were actually a summary account of a more detailed analysis describing work performed under contract with the Meteorology Laboratory of the U. S. Environmental Protection Agency. Mr. Calder wanted to draw attention to the existence of the study and to the final contract report "Validation and Sensitivity Analysis of the Gaussian Plume Multiple-Source Urban Diffusion Model," by R. C. Koch and S. D. Thayer, Geomet, Inc.; Rockville, Md., November 1971. This was available for sale to the public as document N.T.I.S.-PB 206 951 from the National Technical Information Service (NTIS), U. S. Department of Commerce, 5285 Port Royal Road, Springfield, Va., 22151.

The basic model was short-term and steady-state, and used one-hourly average values for the input parameters describing the SO_2 pollution emission rates and the atmospheric meteorological-dispersion conditions. The final report provided details of the necessary algorithms for these short-term estimates and this detail would certainly be required if there was any desire in the future to attempt to standardize air quality models of this type. The basic output from the model was the spatial distribution of one-hourly average SO_2 concentration values. However, algorithms were available to provide statistical properties of these distributions, such as the concentration frequency distributions, long-term average values of concentration, etc. A noteworthy computational feature of the Geomet formulation of the Gaussian plume model was an approximate method for reducing the calculation of two-dimensional integrals that express concentration contributions from area-source emissions distributions to one-dimensional integrals, and the development and use of a statistical sampling plan to reduce the computational burden in calculating concentration frequency distributions.

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VALIDITY OF THE MULTIPLE-SOURCE, GAUSSIAN PLUME URBAN DIFFUSION MODEL USING HOURLY ESTIMATES OF INPUT

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1. INTRODUCTION AND BACKGROUND

Recent emphasis on the development of complex models for treating the transport and diffusion of pollutants in urban areas, on the one hand, and proposals that only very simple models are justified, on the one hand, make it important that the capabilities and limitations of the commonly used multiple-source Gaussian plume model be determined. A study was carried out under sponsorship of the Environmental Protection Agency to critically evaluate the predictive accuracy of this model and to determine its sensitivity to changes in input (Koch and Thayer 1971). This paper describes the validation results obtained in that study. A subsequent paper presented to this Conference describes the sensitivity findings.

Although variations exist in the way the multiple-source Gaussian plume urban diffusion model has been implemented, there is only one basic model. The features of this model have been discussed by several authors and are precisely described by Calder (1970). The basic Gaussian plume equation has been shown to be valid over travel distances of up to a few hundred kilometers (e.g., Slade 1968 and Pasquill 1962). Furthermore, a great deal of experimental work has been devoted to defining parameters for the Gaussian plume model in both rural and urban environments (McElroy 1969). The results reported here describe the validity of using this equation to simulate urban SO_2 concentrations in detail.

2. THE MODEL

A basic assumption in using the Gaussian plume equation to estimate pollutant concentrations in urban air is that the dynamics of the concentration field can be approximated by a sequence of relatively short steady-state periods. During each steady-state period there is a unique mathematical function which describes the concentration(χ) at any receptor location resulting from pollutants emitted by any continuous and constant point source(Q) in terms of the wind oriented receptor coordinates (x,y) relative to the source.

$$\frac{\chi}{Q} = \frac{1}{\pi \bar{u} \sigma_y(x) \sigma_z(x)} \exp\left\{-1/2\left[\frac{y^2}{\sigma_y{}^2(x)} + \frac{h^2}{\sigma_z{}^2(x)}\right]\right\} \quad (1)$$

where $\bar{u}$ = mean wind speed,

$\sigma_y(x), \sigma_z(x)$ = horizontal and vertical diffusion functions, and

h = effective source height.

The x-coordinate is the alongwind distance and the y-coordinate is the crosswind distance between the source and the receptor; both coordinates are defined by a uniform horizontal wind direction which characterizes the steady-state period. In addition, the steady-state period is characterized meteorologically by a horizontally uniform mean wind speed profile (speed may vary with height), a mixing layer depth(L) and a stability. The latter two characteristics determine the parameters of the diffusion functions which have the following form:

$$\sigma_y(x) = ax^p \quad (2)$$

$$\left.\begin{aligned} \sigma_z(x) &= bx^q & x &\le \left(\frac{L}{2b}\right)^{\frac{1}{q}} = x_1 \\ \sigma_z(x) &= L & x &\ge \left(\frac{L}{b}\right)^{\frac{1}{q}} = x_2 \\ \sigma_z(x) &= \frac{x+x_2-2x_1}{x_2-x_1}\left(\frac{L}{2}\right) & x_1 &< x < x_2 \end{aligned}\right\} \quad (3)$$

The parameters a,b,p and q are determined from the stability condition.

Equation (1) above is applicable for non-settling stable pollutants. It may be extended to treat simple removal processes which are characterized by a constant decay rate by multiplying the right hand side by an exponential decay factor, e.g.

$$\exp\left(-\frac{0.693}{t_{50}}\frac{x}{\bar{u}}\right) \quad (4)$$

where t_{50} = half-life of the decay processes.

It is impractical to treat all sources in an urban area individually. Sources whose emission rate is large relative to other sources in its vicinity are treated as point sources. All other sources are treated as an area source having a mean emission rate per unit area which can be specified as a function of horizontal position using appropriate emission inventory techniques. Since an element of the area source $q(x,y)\,dx\,dy$ is a point source, the concentration (χ_a) at a receptor location is obtained by summing the concentrations from all elements upwind of the receptor.

$$\chi_a = \int_0^{\infty}\int_{-\infty}^{\infty} \frac{q(x,y)}{\pi \bar{u} \sigma_y(x) \sigma_z(x)} \exp\left\{-\frac{1}{2}\left[\frac{y^2}{\sigma_y{}^2(x)} + \frac{h_a^2}{\sigma_z{}^2(x)}\right]\right\} dy\,dx \quad (5)$$

where h_a = effective height of the area source.

Since q(x,y) is zero outside the urban area, the fact that the limits on the intergals are actually finite is of no concern. The integral in Equation (5) can be simplified by introducing the "narrow plume" assumption which states that the spatial distances between variations in the area-source emission rate are large compared to the horizontal diffusion parameter σ_y, so that cross-wind variations in q(x,y) may be ignored; let $q'(x) = q(x,0) \sim q(x,y)$. We then have

$$\chi_a = \int_0^{\infty} \frac{q'(x)}{\pi \bar{u} \sigma_y(x) \sigma_z(x)} \exp -\left[\frac{h_e^2}{2\sigma_y^2(x)}\right] dx \qquad (6)$$

which considerably reduces the computational burden. Equations (5) and (6) were compared using numerical evaluation techniques for 10 selected one-hour data periods and found to produce only very small differences. The results quite clearly substantiated the validity of the narrow plume assumption.

3. VALIDATION ANALYSIS

Concentratipns calculated using a computer programmed version of this model were compared with SO_2 measurements obtained in St. Louis and Chicago. Both short-term concentrations for 1 or 2 hours and long-term concentrations for 1 month or 3 months were compared. The model calculations were made for one-hour periods using the best available estimates of hourly means for all model inputs. A determination of the best procedure for estimating each input was made objectively on physical grounds, without regard to whether the procedure would improve or worsen the validation results. No empirical fitting, adjustment or calibration was employed in the model.

3.1 Model Inputs

For each one-hour period wind direction and speed were determined as the vector average of one-hour mean observations from several locations. Although the validation study is based on the use of several wind observations (3 for St. Louis and 8 for Chicago), there is close agreement between the vector average and the nearest airport wind. The validation findings would not be significantly changed by the use of a single airport wind observation. Differences are most frequent with wind speeds less than 5mph. The validity of the model might be decreased at locations where light winds occur frequently if only a single wind observation were available.

An hourly urban diffusion stability index was computed using airport weather observations according to the rules outlined by Turner (1964). For St. Louis the airport weather observations were taken at Lambert Field; for Chicago, Midway Airport. The diffusion parameters in Equations (2) and (3) were determined from the stability index using the results of urban tracer experiments reported by McElroy and Pooler (1968). Hourly estimates of the mixing layer ceiling were interpolated in time and space from mixing layer heights indicated by the closest radiosonde observations. The 12Z observation height was assumed to be valid from midnight to 6a.m. The 00Z observation height was assumed to be valid from 2p.m. to midnight. Linear interpolation was used to estimate heights for the hours between 6a.m. and 2p.m.

Hourly SO_2 emission rates for point and area sources were estimated on the basis of fuel consumption estimates and production process emission rates. Algorithms were developed to relate these estimates to generator output loads, production operating schedules, day of the week, hour of the day, temperature, annual fuel consumption rate and annual process production rate. The algorithms used for St. Louis were primarily developed by EPA personnel (Turner 1968). Those used for Chicago were primarily developed at Argonne National Laboratory (Roberts et al., 1970).

The effective height of point sources in the Chicago data was estimated using the plume rise equations recommended by Briggs (1969) for leveled-off plumes. For the St. Louis data the original stack data was not available; however, plume rise, wind speed products computed from the original data using the Holland formula (Calder 1970) were furnished by EPA for each point source. The available stack data and hourly meteorological observations were used to derive hourly estimates of effective source height (i.e., plume rise plus physical stack height) for each point source. The area sources were assumed to have a constant effective height throughout the data period.

3.2 Results

Comparisons between calculated and measured SO_2 concentrations were used to determine how well the model estimates long-term mean concentrations, the distribution of short-term concentrations over a period of a month or a season, and individual short-term concentrations. Three month mean concentrations were calculated for 10 sampler locations in St. Louis. One month mean concentrations were calculated for 8 sampler locations in Chicago. The resulting calculated and measured long term concentrations are shown in Table 1. The difference in the pairs of comparisons varies from less than 0.01 to 0.20 mg/m^3. The results of a regression analysis of measured on calculated concentrations are shown in Table 2. The correlation coefficients were 0.68 for the St. Louis comparisons, 0.87 for the Chicago comparisons and 0.72 for the two locations combined. The slopes of the regression lines for the three sets of long term concentration comparisons were not different from unity at the 5% significance level.

The long-term concentration comparisons in Table 1 clearly show that the magnitude of the model error (defined as calculated minus measured concentration) varies with the magnitude of the calculated concentration. The ratio of the error to the calculated concentration seems to be the best way to express the nature of the distribution of observed concentrations associated with a model estimate. The mean and range of this ratio are shown in Table 2 for the three sets of long-term concentration comparisons. These results suggest that on the average the model overestimates the long-term mean by 13%. The errors were observed to vary from a 62% underprediction to 67% overprediction over the 18 locations for which comparisons were made.

Table 1. Statistical properties of measured and calculated SO_2 concentrations for ten St. Louis and eight Chicago sampling stations

Location	Long-Term* Mean Concentration (mg/m^3)		Standard Deviation of Short-Term† Concentrations (mg/m^3)			Mean Absolute Difference	Correlation Coefficient
	Measured	Calculated	Measured	Calculated	Difference		
St. Louis # 3	0.16	0.20	0.14	0.18	0.21	0.13	0.20
" 4	0.18	0.14	0.16	0.20	0.21	0.12	0.29
" 10	0.34	0.21	0.24	0.16	0.26	0.20	0.24
" 12	0.18	0.21	0.14	0.21	0.19	0.12	0.46
" 15	0.14	0.12	0.13	0.12	0.13	0.09	0.45
" 17	0.21	0.18	0.12	0.16	0.16	0.11	0.39
" 23	0.09	0.19	0.11	0.24	0.24	0.14	0.25
" 28	0.09	0.09	0.12	0.15	0.15	0.08	0.36
" 33	0.07	0.06	0.09	0.10	0.10	0.05	0.40
" 36	0.08	0.09	0.08	0.13	0.12	0.06	0.44
Chicago # 1	0.03	0.05	0.06	0.11	0.10	0.04	0.47
" 2	0.11	0.10	0.09	0.11	0.13	0.09	0.15
" 3	0.31	0.38	0.15	0.42	0.40	0.22	0.30
" 4	0.12	0.32	0.09	0.29	0.27	0.20	0.37
" 5	0.06	0.13	0.05	0.14	0.14	0.08	0.28
" 6	0.02	0.06	0.03	0.10	0.10	0.04	0.18
" 7	0.10	0.16	0.10	0.16	0.16	0.10	0.32
" 8	0.04	0.04	0.04	0.08	0.08	0.04	0.07

* 3 months for St. Louis, 1 month for Chicago.

† 2 hours for St. Louis, 1 hour for Chicago.

Table 2. Properties of comparisons between calculated and measured concentrations

Type	Location	Regression of Measured on Calculated Concentration			Ratio of Error* to Calculated Concentration		Number of Comparisons
		Correlation Coefficient	Slope	Intercept	Mean	Range	
Short-Term	St. Louis	0.35	0.31	0.11			9420
	Chicago	0.49	0.25	0.06			5407
Long-Term	St. Louis	0.68	0.98	0.00	-0.04	-0.62 to 0.53	10
	Chicago	0.87	0.63	0.00	0.34	-0.10 to 0.67	8
	Both	0.72	0.69	0.02	0.13	-0.62 to 0.67	18

* Error is defined as calculated minus measured concentration.

In order to determine how well the model estimates the distribution of short-term concentrations over a long-term period, for each location the sets of calculated and observed concentrations were divided into 10 class intervals. A chi-square test was used to determine if the frequency of occurrence of the class intervals were significantly different. As a result of these comparisons it was concluded that calculated and observed distributions were in reasonably good agreement. The standard deviations of the calculated and measured concentrations for each location are shown in Table 1. Each standard deviation is based on 700 to 1000 values. As a result all but two pairs of measured and calculated values are different at the 5% significance level when judged on the basis of an F test. However, the magnitude of the difference is not large for several pairs which show significant differences.

Three statistics are presented to show the validity of paried comparisons of calculated and measured concentrations at individual short-term periods (2 hours for St. Louis, 1 hour for Chicago). The standard deviation of the difference over the long-term period, the mean absolute difference, and the correlation coefficient are shown for each of the 18 locations. The standard deviation of the difference between calculated and measured concentrations varied from 0.08 to 0.40 mg/m^3 compared to a range in the calculated long-term means of 0.04 to 0.38 mg/m^3.

The mean absolute difference varied from 0.04 to 0.22 mg/m^3. The correlation coefficient varied from 0.07 to 0.44. The overall correlation between calculated and measured short-term concentrations is shown by the regression analysis results presented in Table 2. For St. Louis the correlation coefficient is 0.35; for Chicago, 0.49. The distribution of errors observed in these comparisons is summarized in Table 3. It may be noted that the frequency of occurrence of the various error magnitudes is similar for the two locations. Approximately 50% of the model estimates were within ± 0.05 mg/m^3 of the measured values; however, over 20% of the estimates differed from the measured values by ± 0.15 mg/m^3 or more.

Table 3. Comparisons of error distributions for short-term concentration estimates at St. Louis and Chicago

Range of Predicted Minus Observed Concentration mg/m^3	% of Comparisons Within Error Limits	
	St. Louis (Mean Observed Concentration = 0.15 mg/m^3)	Chicago (Mean Observed Concentration = 0.10 mg/m^3)
± 0.01	15	17
± 0.02	25	30
± 0.05	46	53
± 0.10	65	73
± 0.15	76	82

The model is clearly more acceptable in making long-term mean estimates and in defining the distribution of short-term concentrations over a long-term period than in estimating short-term concentrations for a specific time. It is likely that the ability to accurately estimate emission rates for specific time periods has a considerable impact on the model accuracy. Over a long-term period, errors in emission estimates are likely to average out, but at any individual time large errors are likely to occur.

3.3 Use of a Sampling Plan

In most previous approaches to computing long-term concentrations it has been assumed that emission rates are independent of meteorological conditions, and the long-term average concentrations were calculated using a mean emission rate. This assumption was necessitated by the lack of data available to estimate diurnal variations. In the more detailed approach used in this study all hourly concentrations within a long-term period are calculated to determine the long-term mean and the frequency distribution of short-term concentrations. This requires a considerable computational burden. It is desirable to introduce a computational procedure which does not bias the correlation between emission rates and meteorological conditions and does not require excessive computation time. An approach to reducing the running time by statistical sampling of a calendar-time-oriented input set has been developed based on proportionate stratified sampling (Hansen et al. 1953). In the proposed plan the hours are statistically sampled by randomly selecting the first hour of the first day in the set, and selecting additional hours which are one sample increment away from the selected hour, as follows: The first hour is incremented by one for each succeeding day in the calendar period. Thus, if the sample increment is six hours and the first selected hour is hour 1, hours 1, 7, 13, and 19 will be selected from the first day; hours 2, 8, 14, and 20, from the second day; etc.

In order to test the validity of the use of various sampling intervals, the sampling plan was applied to the St. Louis data at each of the 10 stations for which hourly calculations had been made for the months of December 1964, January and February 1965. The mean, standard deviation and deciles of hourly concentrations were obtained with statistical sampling intervals of 2, 4, 6, 8, 12, and 24 hours. The largest deviation of a decile concentration for a 24-hour sampling interval, from that obtained with a one-hour sampling interval, was 25 percent of the one-hour decile value. In absolute magnitude the greatest deviation was 601 μg/m^3 compared to 513 μg/m^3 for the one-hour 90 percent decile at station number 12. The results show that, except for the single highest value, the entire frequency distribution of concentrations can be reasonably reproduced using a 24-hour interval between sampled periods. In the view of the uncertainties in the model predictive accuracy on an hour-by-hour basis shown by the comparisons between predicted and observed concentrations, the small errors in constructing frequency distributions by using the selective 24-hour sampling plan illustrated here are not significant.

4. CONCLUSIONS

The results presented here are based on the predicted and observed concentrations of SO_2 at eight locations in Chicago during January 1967 and 10 stations in St. Louis during December 1964 to February 1965. The predictions used hourly estimates of meteorological and emission parameters. The atmospheric stability was estimated from hourly weather observations from an adjacent airport using the McElroy-Pooler diffusion parameters based on Turner's definitions of stability categories. The mixing layer ceiling was estimated from radiosonde observations taken twice daily from remote locations (100 to 200 miles away). The wind speed and direction were hourly averages of several (3 in St. Louis, 8 in Chicago) continuous records. The emission rates of the largest sources were identified and located individually. For other sources a mean emission rate per unit area was estimated for a square gridwork of points with a one mile spacing between adjacent points. Each emission rate was related to hourly estimates of space heating and other operating requirements. Calculated long-term (month or season) concentrations averaged over several locations are in good agreement with measured concentrations. Calculated short-term (one or two hours) concentrations at individual stations show larger deviations from measured concentrations than do the long-term calculations. However, over a period of a month, or a seasons, the overall distribution of calculated short-term concentrations closely approximates the distribution of measured concentrations. Proportionate stratified sampling is an effective method of selecting a limited set of short-term periods which adequately define a representative distribution of short-term concentrations in a long-term period. One hour out of 24 is a sufficient sample size for a three month period if the selected hour is varied to include all hours of the day.

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SENSITIVITY ANALYSIS OF THE MULTIPLE-SOURCE GAUSSIAN PLUME URBAN DIFFUSION MODEL

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1. INTRODUCTION

The companion paper to this one, on the validity of the multiple-source Gaussian plume urban diffusion model, describes a carefully defined fundamental short-term steady-state Gaussian plume urban diffusion model, and its various modes of implementation, and presents the results of validation analyses which compare its predictions with SO_2 observations.

It is important to understand the sensitivity of a model's output to its input for a variety of reasons: if the model is a valid one, i.e., representative of reality, then we can use sensitivity results to better define and understand the real-world parameters which dominate the process; further, we thus pinpoint the parameters which may require further study and better understanding, and on which to focus our data collection efforts. Having previously examined the model's validity in the companion paper to this, we now look at that model's sensitivity to its input parameters.

This paper presents selected principal results of an extensive analysis of the sensitivity of that model to model input parameters. A reasonable range of values of interest were selected for each model input, and combinations of values of all input parameters were selected for use in testing for sensitivity. Extensive exercising of the computer model using many thousands of combinations of input values delineated and excluded the areas of insensitivity, and focussed attention on the sensitive areas, which were then subjected to further analysis to characterize the dependencies in quantitative fashion. The analysis demonstrates the insensitivity of the model-predicted concentrations to the parameters of the distribution of area source emission heights and wind speed profile parameter value.

This paper presents a quantitative description of the sensitivity of the model to the following parameters: changes in spatial variability in emissions; the vertical diffusion parameter σ_z; the pollutant's half-life; the wind speed; the mixing ceiling; and the wind direction.

2. THE MODEL, ANALYSIS CONCEPTS, AND PARAMETERS STUDIED

2.1 The Multiple-Source Gaussian Plume Urban Diffusion Model

The most commonly used meteorological model is based on the steady-state Gaussian plume concept and lies, in complexity, somewhere between the simple box model and the Gaussian puff trajectory model. Although variations exist in the way this model has been implemented, there is only one basic Gaussian plume model. The generality of this model and its application to urban diffusion analysis has been described by Calder (1970). This basic model has been shown to be valid over downwind travel distances of up to a few hundred kilometers (e.g., see Slade (ed.), 1968 and Pasquill, 1962). Since 1 to 50 kilometers is the distance scale of primary interest in studying urban air pollution problems and since a great deal of experimental work has been devoted to defining parameters for the Gaussian plume, this concept has been the principal one used to analyze urban air pollution problems.

The calculations employ the "narrow plume" assumption to compute atmospheric pollutant concentrations from the area sources involved, and the McElroy-Pooler diffusion parameters based on Turner's definitions of stability categories to represent the diffusion parameters σ_y and σ_z.

The calculations use hourly estimates of meteorological and emission parameters. The atmospheric stability is estimated from airport weather observations. The mixing layer ceiling is estimated from standard radiosonde observations (100 to 200 miles away). The wind speed and direction are hourly averages of several continuous records. The largest sources are treated as points. A mean emission rate for each square mile is estimated for other sources. Each emission rate is related to hourly estimates of space heating and other operating requirements. No "calibration" or other adjustment of the inputs or output concentrations is employed anywhere in the analysis.

2.2 Sensitivity Analysis Concepts

Sensitivity is formally defined as the partial derivative of a model's output with respect to its input. In the case of complex models, however, a more practical definition, which is often employed for analytical purposes, is the incremental change in output resulting from an incremental change in input.

In a numerical simulation model as complex as the one utilized in this report, it is not possible to study all aspects of sensitivity analytically, nor is it safe to infer sensitivities from the form of the Gaussian model, which is the kernel of the simulation, because of the numerous interactions involved. Proper analyses required appropriate numerical exercising of the complete simulation.

Sensitivity analyses of urban pollution models have been reported by Hilst (1970) and Milford, et. al. (1970a; 1970b). Hilst applied sensitivity analysis concepts in an example case study of the TRC Region Model, developed for the State of Connecticut, which involved a combination of a trajectory-oriented Gaussian model with the puff version for area sources and the plume version for major point sources. Hilst's results are of interest, but as he attests, limited in scope by the case study nature of the analysis.

The work reported by Milford, et. al., deals with the variations of the model developed for the New York/New Jersey/Connecticut Air Quality Region. The studies which they have reported describe a model which bears a general resemblance to the steady-state plume model implemented in the study covered in this report. Their work, however, is very specifically oriented in form, input, and application to the greater New York area, and their reported sensitivity results focus largely on highly specific individual case examples, rendering useful generalizations difficult. The study in this report attempts to derive broad-scale significant sensitivity findings from a generally applicable model.

This paper describes the work performed to analyze the sensitivity of the output concentrations of the multiple-source Gaussian plume diffusion model to model input parameters. The analysis concentrates on the sensitivity of the short-term version of the model, with reference to the longer term climatological version where appropriate. The parameters and their ranges are discussed, the methodology is described, and the analysis and results are presented.

2.3 Parameters Investigated

2.3.1 Parameter Framework

In order to design model sensitivity experiments, it is necessary to define a reasonable range of interest for each model input and to select combinations of values of all input parameters to use in testing for sensitivity. It was found that the inputs could be represented by a small number of values scattered over the total range of values of interest.

Sensitivity analysis in this program was focussed on changes in calculated concentrations which are associated with changes in input for a given set of input values. In view of the large number of such comparisons which are possible in the context of the total sensitivity study, the first step was to define reasonable ranges of interest for each parameter; subsequently, determination was made of which parameters have little influence on output over their defined range of values, and the remaining parameters were analyzed in more detail.

The parameters were ordered, fo analysis purposes, into a framework which defined them as related to the emission-receptor environment, the pollutant's characteristics, or the meteorological environment. The emission-receptor class included: area source grid dimensions or spacing, degree of aggregation of point sources into area sources, assumed emission heights for area sources, receptor locations, and treatment of diurnal variations in emissions. Only one pollutant characteristic was considered, that of any apparent depletion of pollutant which can be represented by an exponential decay process. The meteorological environment parameters were: the wind speed and wind profile power, wind direction, height of the mixing ceiling, and the diffusion function and stability class.

The initial set of parameters and the specific input values selected for the pollutant characteristics and meteorological environment are discussed below. The values selected were based on the judgement and experience of the in-house staff of diffusion meteorologists, as well as, to some extent, on the numerical information developed in the course of the companion validation study.

- o Decay Half-Life: One obvious choice is for no decay (infinite half-life); the other (30 minute half-life) represents a moderately reactive material. (A third extremely short half-life (5 minutes) was experimented with to a small degree).
- o Wind Speed: Three values (2,6 and 18 m/sec) are intended to reflect light, moderate and strong anemometer-level winds.
- o Wind Profile Power: Two values, (0.15 and 0.3) arbitrarily chosen as depicting the range (0.10-0.50).
- o Wind Direction: (See Sections 2.3.2 and 4.3.2).
- o Mixing Ceiling: A very low value (100m) an intermediate (characteristic) value (500m) and a high value (2500m).
- o Diffusion Function and Stability Class: The three cases represent extreme atmospheric stability (Pasquill class E), neutral stability (McElroy-Pooler class D), and extreme instability (McElroy-Pooler class 1).

The variations in the emission-receptor environment are discussed in Sections 2.3.2 and 4.1.

2.3.2 Generalized Emission Pattern

For a study of this type, there is a need to define a selection of basic geographic patterns of emission rates, as well as the selection of receptor locations relative to this pattern at which to measure sensitivity affects. It seems reasonable to define three principal, general situations concerning the relationship of a receptor relative to an emission pattern:

1. The receptor is in an area of relatively uniform emissions with no significantly strong upwind sources (upwind receptor).

2. The receptor is in an area of high emission rates surrounded by noticeable lower upwind emission rates (as in the center of urban area), (center receptor).

3. The receptor is in area of light or moderate emissions with significant upwind sources (downwind of urban center), downwind receptor).

In the validation analysis (see our companion paper) the relative contribution to the total emissions arising from point sources, in contrast to area sources, had already been defined for the receptor locations which represent sampling stations. From these results it was noted that, in by far the majority of the cases examined, the overall contribution from point sources was small. There were notable exceptions in which the point sources were the dominant contributors to particular receptor locations under particular conditions. The impact of such special situations is examined further in Section 4.3.2. Meanwhile it was determined that the first order of importance was to examine realistic (and, hopefully, generalized) patterns of area source emissions, in order to assist in the definition of emission rate patterns and the associated receptor locations for use in the sensitivity analysis.

The area source emission rates for each square mile and each hour in a 2036-hour St. Louis data sample had been previously stored on magnetic tape for use in the validation analysis. These data were retrieved and used to generate hourly contour maps of the area source emission rates, which were then studied to determine whether consistent patterns were present. From this study, one can make the general observation that, although the magnitude of emissions at any point may vary by a factor of as much as ten, the distribution of the pattern remains relatively consistent. No outstanding variation in the general shape of the pattern was noted with time of day or day of week. As a result, it was decided that the three receptor location characteristics described above (upwind, center and downwind) could be reasonably represented by a single emission pattern with three such receptor locations. The selected pattern is shown schematically in Figure 1. The principal wind direction was defined to be from 349° as shown (changes in direction to 020° are examined in Section 4.3.2), and the three large X's were selected as receptor locations representing upwind, center (high emission), and downwind receptor zones. The solid contours represent area emission rates in grams per second per square mile. The small dots and circles represent individual point sources, and are discussed in Section 4.1.2.

The sensitivity analysis was therefore performed in the context of this representative background pattern of emissions, and the parameters considered were varied against this background. While this is a specific case, it is considered to be rather generally applicable to many urban situations; further, it has the advantage of enabling focus on a wide variety of specific questions of emission patterns sensitivity, by considering the three receptors with the two alternative wind directions in various combinations.

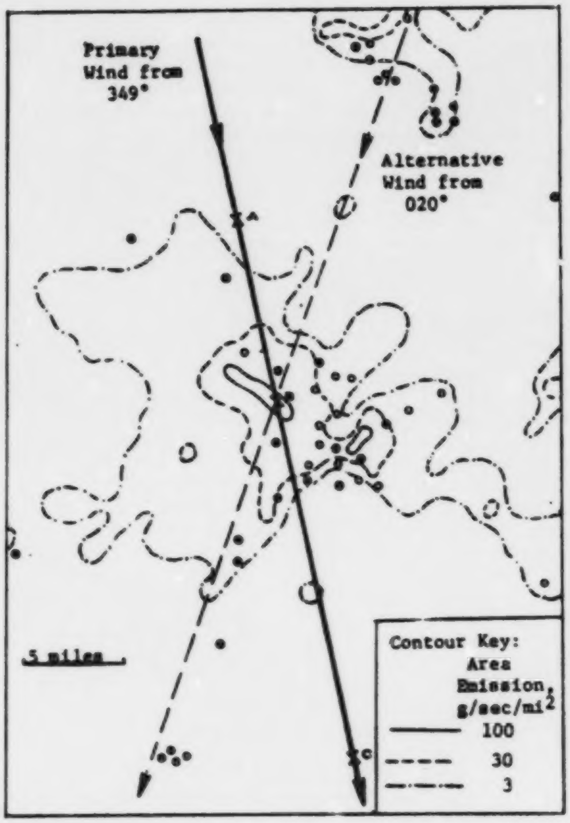

Figure 1. Generalized Area Source Emission Contours (See Key). Receptor Points are A (Upwind), B (Center) and C (Downwind). Black Dots are Highest 19 Point Source Emitters; Circles Represent Next Highest Group.

3. ANALYSIS METHODOLOGY

The methodology followed is on in which changes in input are used to define changes in output. The output changes are then examined as relative or absolute changes and ranked to determine those which are most significant. Short-term concentrations are emphasized in the analysis. The first step in the analysis consisted of computer runs representing a full factorial replication of all combinations of the inputs which are relevant to short-term concentrations. This includes all but wind direction and the magnitude of diurnal variations in emissions, which are treated separately. The total number of combinations is 5832 (i.e., 2 pollutant half-lives x3 wind speeds x2 wind profile powers x3 mixing ceilings x3 diffusion functions x3 sets of point sources x3 area source grid spacings x2 sets of emission heights for area sources x3 receptor locations). Within this total, for each model input, two to three thousand sets of variations (depending on the input parameter involved) in model output were therefore generated for each specified variation in input.

Inputs which showed little output variation over all sets, or almost all sets, were accordingly identified as insensitive inputs, and variation in these insensitive parameters was not considered further. Each of these is discussed in Section 4. The selection of a criterion which would represent a significant change in output over a range of input values was governed by the validation findings. As a result of those findings, it was decided that input changes must generate at least a 50 percent change in output for the range of input values considered in order to qualify as a significantly sensitive input. Where significant change was found, the analysis was pursued in greater depth, as is described in Section 4.

4. RESULTS

In the following discussion, the results of the analyses of the computer runs described in Section 3. are presented in detail. The analytical procedure for defining the impact of each input parameter consists of identifying "sensitive" changes in calculated concentrations resulting when an input parameter is varied. A "sensitive" change is defined to be a change in the input parameter which results in a greater than 50 percent change in the calculated concentration. Such cases are then subjected to more detailed analysis.

4.1 Emission-Receptor Environment

4.1.1 Area Source Grid Spacing

Urban diffusion modelers usually identify only the most significant point sources, and obtain reasonably accurate estimates of emission rates for these sources. Emissions from other sources are treated as uniformly distributed over a segment of area, and estimates of the emission rate per unit area are mde for such convenient squares or blocks of the urban area. A square mile is a frequently used block size. For sensitivity purposes variation in the fineness of the area source representation is accomplished by changing the spacing between grid points and the corresponding block size in the area source emission inventory. The two questions of concern here are, What is the real spatial variability in emission rates? and, How accurately should the real spatial variability be reflected in the model? Since the real spatial variability is not known, except as estimated for square mile blocks, this parameter has been hypothesized for testing sensitivity, thus enabling definition of the conditions under which sensitivity occurs. The assumption has been made that when a unit square mile area is divided into 16 quarter-mile squares, the emission rate per unit area for each subdivision will be approximately normally distributed (in a statistical, not geographical, sense) about a mean value with a standard deviation equal to one-half the mean. In the sensitivity analysis, mean values for square mile areas were used with a random number generator to define emission rates appropriate to the smaller quarter-mile squares. Standard IBM computer routines for random number generation and inverse normal function evaluation were used.

The basic computer model and the selected set of SO_2 emission data drawn from the St. Louis data sample were used to test whether changing the grid resolution (1 mile) to a finer (0.25 mile) or a coarser (4 mile) mesh had a significant effect on the calculations.

Parenthetically, it will be seen that, when the initial large-scale screening analysis was performed, two parameters were immediately demonstrated to have only insignificant effects on the output concentrations. These two, the vertical distribution of area source emissions (4.1.3) and the wind profile power (4.3.1) were accordingly eliminated from the analysis in considering sensitivity to other inputs; at the same time, it was found possible to reduce the number of mixing ceilings considered (Section 4.3.3) from three (100, 500 and 2500m) to two (100 and 500m) for most of the detailed comparisons. Thus, the number of combinations considered in this section was reduced from 5832 to 972 (i.e., two pollutant half-lives x3 wind speeds x1 wind profile power x2 mixing ceilings x3 diffusion parameters x3 sets of point sources x3 area grid spacings x1 area source emission height x3 receptor locations). Of these, 324 represent the effect of a changing grid mesh size as a function of meteorological conditions in the presence of the standard of a maximum of 51 individually identified point sources.

When the 324 are examined in detail, almost half of the cases (141 cases or 47%) show significant changes in concentration (40% change) when the one-and four-mile spacings are compared. Similarly, 78 cases (24%) show significant changes when the 1- and the 0.25-grid sizes were compared. When a shift in wind direction to 020° was considered, as shown in Figure 1, the number of sets yielded significant changes with a change in grid mesh size was reduced only slightly, implying no change in the demonstrated sensitivity.

These results show that averaging area source emission rates over areas larger than 1 square mile can lead to significant errors in estimated pollutant concentrations. Furthermore, if the standard deviation in emission rates of quarter mile squares (about 6 city blocks) is of the order of 50 percent of the mean over a square mile area, (as postulated in the beginning of this section), then even the use of square mile average emission rates can lead to significant errors in estimated pollutant concentrations.

4.1.2 Aggregation of Point Sources into Area Sources

As a further sensitivity test, the effect of various levels of aggregation of point source emission data into the general area source emission rate was examined. This was done by comparing calculations when all (51), some (19), or none of the major sources were merged. The top nineteen point sources emit SO_2 at rates ranging from 277 to 2680 g/sec, at least as of the 1964 inventory used here. The figure of nineteen arises because, in addition to the two extreme cases of merging none, or all, of the point sources, the effect of merging just those points whose emission rates were less than 10 percent of the largest emission rate, was examined (i.e., merging all but the highest 19 emission rates). The location of the point sources relative to the three sensitivity receptor locations is shown in Figure 1. In order to examine the effect of large point sources on the center receptor location, the wind direction was shifted as indicated in Figure 1 to see what effect that would have on the sensitivity results.

Now, considering the impact of merging point sources into the area sources, recall that this examination focuses primarily on the overall impact of such changes, rather than on the fine scale details of effects on specific receptors in the vicinity of significant point sources. The latter aspect is dealt with by Milford, et. al. (1970a), and, because of its wind direction dependence, in Section 4.3.2 of this report. In the broader context, then the following findings apply. For the smaller grid sizes (1 and 0.25 miles) only a negligible number (1-4%) of the calculated concentration cases show significant changes when the number of individual point sources is reduced first from 51 to 19, and then to zero. For the coarser 4-mile grid, we find 4 percent of the cases showing significant concentration changes when the 19-source case is compared to the 51-source case, with an increase to 18 percent when the "no-point-sources-considered" case is thus compared.

Therefore, we see that the broad-scale concentration picture is little affected either by treating individually, or by merging, various numbers of point sources when the area source grid scale is of the order of 1 mile or smaller; however, with a larger grid scale (of the order of 4 miles), failure to take into account at least the main point sources individually can cause problems. The 4-mile grid dimension was already questionable, of course, from the previously stated findings on grid size alone (Section 4.1.1).

4.1.3 Vertical Distribution of Area Source Emissions

Area source emissions of SO_2 consist of a large variety of individual sources including stores, small plants, apartment buildings and small single and multi-family homes, to mention a few of the more common types. Since the emissions from these sources are primarily contained in burned fuel exhaust, the emissions are hot. As a result, the emissions are released from a variety of heights with a variety of plume rise effects.

In the sensitivity analysis, the results obtained by allocating 25 percent of the area emission rate to a height of one-half the mean emission height, and 25 percent to one and one-half times the mean emission height (leaving 50% emitted at emission height), are compared with those when all emissions in a given area are at the same height. In terms of the initial set of 5832 input combinations there were 2916 pairs of such comparisons. In none of these was the concentration resulting from one distribution of heights 50 percent greater than that from the other. In fact, only in the case of a combination of high decay rate, low wind speed, and stable diffusion parameters, did one exceed the other by more than 25 percent. In general, the difference between the vertical distributions was negligible. As a result, in additional calculations, all emissions in any given area source were treated as emanating from a single height.

4.1.4 Diurnal Variation in Emission Rates

The sensitivity of the model to diurnal variations in SO_2 emission rates is given a separate, qualitative evaluation in this section, by analyzing the factors which affect the emission rate estimations. It was found that errors in reported annual or seasonal emissions from particular sources will result in porportionally systematic errors in calculated diurnal variations in concentrations in the vicinity of the emission error. Because the emission algorithms are temperature based, unseasonable temperatures, or sudden atmospheric temperature changes will result in corresponding systematic errors in predicted short-term concentrations at all locations for a short lag period, until an adjustment in space heating operations occurs. Over a long-term period errors in short-term concentrations due to differences between actual and estimated emission rates will tend to be balanced out.

4.1.5 Receptor Location

The receptor locations studied are discussed in Section 2.3.2. The parameter of receptor location impacts extensively throughout the analysis results, interacting with the parameters of pollutant half-life, wind speed, wind direction, mixing ceiling and diffusion function. Accordingly its effect is demonstrated in detail as applicable in each of the sections (4.2 and 4.3) which cover those interacting parameters.

4.2 Pollutant Characteristics

4.2.1 Pollutant Half-Life

The effect of pollutant half-life due to exponentially represented atmospheric removal processes on short-term model (one-hour) concentrations was examined to determine whether it was significant, and, if so, under what conditions it was most significant. A total of 486 pairs of model inputs representing no decay and a one-half hour half-life (486 of each) were compared to examine this question. These consisted of the 972 selected combinations discussed in Section 4.1.1.

From these pairs it is found that a 30-minute half-life (a decay rate of 0.0231/min) causes a significant reduction in concentration in 45 percent of the cases. The most pronounced of these many cases are associated with relatively light wind speeds (e.g., 2 m/sec), and a receptor location which is located significantly downwind of the high emission area. The 30-minute half-life resulted in concentration reductions by a factor of 50 (98%) in the most extreme case. A selected tabulation showing variations in the effect of the decay rate with receptor location and wind speed is given in Table 1, for a 100-meter mixing ceiling with the Pasquill Class E (stable) diffusion parameters. Alternatively, for a 500-meter mixing ceiling, with the McElroy-Pooler Class 1 (unstable) diffusion parameters, the absolute concentrations are reduced by factors of three to six below those shown in Table 1, but the sensitivity pattern as a function of half-life is almost identical.

These results show that the existence of a noticeable depletion process can have a significant effect on concentrations in the low wind situation. This effect will be especially pronounced downwind of high emission rate areas, where the effects are quite noticeable, and even appear at high wind speeds. Other effects of pollutant half-life are evidenced in the discussions of interactions with each meteorological parameter in Section 4.3.

Table 1. Model Concentrations with and without a 30-Minute Half-Life (with a 100m Mixing Ceiling and Pasquill Class E Diffusion Parameters) (1)

Input Parameters		Model Concentrations ($\mu g/m^3$)	
Receptor Location	Wind Speed (m/sec)	With 30-min. half-life	Without Decay
Upwind	2	7	11
	6	3	4
	18	1	1
Center	2	1146	1259
	6	478	547
	18	174	182
Downwind	2	41	2061
	6	145	687
	18	134	229

(1) All Concentrations computed using Figure 1 area emissions with 51 point sources, area grid mesh of 0.25 miles, a single area source height, and a wind profile power law of 0.15.

4.3 Meteorological Environment

4.3.1 Wind Speed and Profile Power Law

The sensitivity of the model to wind speed measured in the city was divided into two components: the wind speed at a reference height of 20.8 meters (a convenient and representative height which corresponded to some available data), and the power which defines the vertical profile of wind speed according to the relationship:

$$u = u_1 \left(\frac{h}{z_1}\right)^p \qquad (41)$$

where

u = wind speed at height h

u_1 = reference wind speed at height z_1

p = power which is a function of atmospheric stability.

In the initial set of 5832 combinations of model inputs defined for the sensitivity analysis there were 2916 pairs of comparisons in which all model inputs were identical except that the power varied from 0.15 to 0.30. In none of these comparisons did the resulting concentrations vary by as much as 10 percent. As a result, this parameter was eliminated from further sensitivity consideration and a value of 0.15 was adopted as the standard value.

In the absence of decay and plume rise the insensitivity of concentrations to the power law parameter makes it clear that the model concentration is inversely proportional to wind speed. This can also be clearly seen in the model formulations. However, the inclusion of a decay constant complicates the relationship. At the upwind and center receptor locations the effect of decay is to slightly reduce the inverse relationship. At the downwind location, the existence of decay causes a reversal in the wind speed relationship over the light to moderate wind speed range (2 to 6 m/sec). These effects are demonstrated by the results presented in Table 2.

Table 2. Model Concentrations as a Function of Wind Speed with a 30-min. Half-Life for Selected Combinations of Model Inputs(1)

a. When the Mixing Ceiling is 100m

Input Parameters		Model Concentrations (ug/m^3)		
Diffusion Function	Wind Speed (m/sec)	Upwind	Center	Downwind
Pasquill, Class E	2	7	1146	41
	6	3	478	145
	18	1	174	134
McElroy-Pooler, Class D	2	4	819	37
	6	2	347	147
	18	1	127	136

b. When the Mixing Ceiling is 500m(2)

Pasquill, Class E	2	7	1143	36
	6	3	476	109
	18	1	173	100
McElroy-Pooler, Class D	2	2	554	11
	6	1	214	32
	18	0	76	29

(1) All concentrations computed using area emission data of Figure 1, 51 point sources, area grid mesh of 0.25 mi., single area source height, wind profile power 0.15.

(2) All column headings of Table 2.a carry through to Table 2.b.

4.3.2 Wind Direction

The influence of wind direction is most critical with regard to specific receptor locations which may or may not be influenced by a strong upwind source, depending on small variations in wind direction. Thus, receptor locations in the center of a strong emission area are equally affected by all wind directions, while locations outside a strong emission area are strongly influenced by whether they are directly downwind of the high emission area.

The effect of various possible errors in wind direction on short-term concentrations was tested using the emission discussed in Section 2.3.2 (Figure 1). The effect of errors in the wind direction estimate of 3, 10 and 45 degrees was examined for the two wind directions shown in Figure 1. The error was allowed to vary to either side of the true direction, and the absolute values of the resulting errors in concentration were averaged for summarizing purposes.

Table 3 contains selected results for the case where all sources (area and point) are considered, and the wind is first taken to be from 349° (Table 3a) (few large upwind point sources; see Figure 1), and then from 020° (Table 3b) (many large upwind point sources). The other fixed conditions are a neutral atmospheric stability and a 500 meter mixing ceiling. The results for the 349-degree direction (Table 3a) demonstrate the variations in model concentration which can occur with various values of wind error, and show the change in effect of such an error depending upon the specific receptor location considered. Errors can go as high as about 25 percent at the central receptor, and up to 100 percent at the downwind location. Note that the pattern is consistent at the downwind location (increasing concentration error with increasing wind error), but not at the central site. Changes in the stability condition (to unstable, or to stable) and/or the mixing ceiling (to 100m) show different absolute values of concentration and error, but quite similar patterns. The results in Table 3b for the 020° direction should be interpreted bearing in mind that this wind shift consideration transfers the relative locations of the up- and downwind sites to some extent in the acrosswind direction (see Figure 1). Errors at the central site can now become significantly larger (up to about 70%) because of the significant upwind point sources, and the other two sites show increased errors, with the "downwind" site losing the consistent increase in error with increased direction error with increased direction error which it had in Table 3a.

These results show the extreme variability of this effect, and the importance of obtaining a representative wind direction to enable adequate definition of the individual short-term concentrations at certain specific types of site locations.

Table 3. Model Concentrations with Various Degrees of Error in the Wind Direction Estimate for Selected Combinations of Model Inputs(1)

a. When the Wind Direction is 349° (see Fig. 1)

Input Parameters		Model Conc. (μg/m³), No Wind Error	Absolute Error in Conc. (μg/m³)		
Receptor	Wind Speed, m/sec		Wind Error		
			3°	10°	45°
Upwind	2 6 18	3 1 0	0 0 0	1 0 0	28 9 3
Center	2 6 18	603 201 67	76 25 8	73 24 8	143 48 16
Downwind	2 6 18	469 156 52	80 27 9	227 76 25	445 25 49

b. When the Wind Direction is 020° (see Fig. 1)(2)

Upwind	2 6 18	7 2 1	12 4 1	18 6 2	75 25 8
Center	2 6 18	1055 352 117	227 76 25	716 239 80	308 103 34
Downwind	2 6 18	23 8 3	18 6 2	154 51 17	125 42 14

(1) All concentrations computed with the area emissions of Figure 1, 51 point sources, area grid mesh 0.25 miles, single area source height, wind profile point 0.15, neutral atmospheric stability, mixing ceiling 500, and no decay.

(2) All column headings from Table 3.a carry through to Table 3.b.

4.3.3 Mixing Ceiling

The sensitivity of model concentrations to changes in the mixing ceiling was examined using mixing ceilings of 100, 500 and 2500 meters. Effects associated with 486 pairs of comparisons of 100- and 500-meter ceiling heights were examined based on the 972 input combinations obtained as described in Section 4.1.1. The most pronounced influence was observed for diffusion parameters associated with unstable meteorological conditions (McElroy-Pooler, Class 1). The least pronounced influence was observed for diffusion parameters associated with stable meteorological conditions (Pasquill, Class E). The least pronounced influence considering receptor location was seen at locations where minimal travel from the principal effective source region was involved. These effects may be clearly discerned in the selected results listed in Table 4. In addition to the 100- and 500-meter mixing ceilings, limited results involving a 2500-meter ceiling have been added for the downwind receptor. These results show that under stable conditions the increased mixing ceiling has no effect, but that under neutral and unstable conditions a noticeable effect occurs. These results suggest that, at downwind locations where significant travel from the primary emission area is involved, the concentration is nearly inversely proportional to the mixing ceiling. With increasingly stable diffusion parameters this effect is reduced until with the stable type of diffusion parameter the effect of the mixing ceiling is negligible.

Table 4. Model Concentrations as a Function of Mixing Ceiling, with a Wind Speed of 6 m/sec for Selected Combinations of Model Inputs(1)

a. When There is no Decay

Input Parameters		Model Concentration With a Mixing Ceiling of:		
Diffusion Function	Receptor Location	100m	500m	2500m
Pasquill, Class E	Upwind	4	4	-
	Center	587	545	-
	Downwind	687	509	509
McElroy-Pooler, Class D	Upwind	3	2	-
	Center	402	234	-
	Downwind	698	147	67
McElroy-Pooler, Class 1	Upwind	3	1	-
	Center	425	173	-
	Downwind	748	175	38

b. When the Pollutant Half-Life is 30 Min.(2)

Pasquill, Class E	Upwind	3	3
	Center	478	476
	Downwind	145	109
McElroy-Pooler, Class D	Upwind	2	1
	Center	347	214
	Downwind	147	32
McElroy-Pooler, Class 1	Upwind	2	1
	Center	364	158
	Downwind	162	41

(1) Concentrations computed using the area emissions of Figure 1, 51 point sources, area source grid mesh of 0.25 mi., a single area source height, and a wind profile power of 0.15.

(2) All column headings of Table 4.a carry through to Table 4.b, except 2500m mixing ceiling.

4.3.4 Vertical Diffusion Parameters

One way of expressing a basic hypothesis of this model (the narrow plume concept), which was found to be acceptable in the model implementation, is that the scale of variability in emission rates (i.e., crosswind distance between significant changes in emissions) is large relative to the scale of variability in plume concentrations (i.e., the diffusion parameter σ_y). Furthermore, as was seen in Section 4.1.2, the contribution of point sources relative to that from area sources is significant only a small percentage of the time, at least in terms of the broad concentration picture. As a result, the crosswind diffusion parameter is of only minor interest in the model. The impact of atmospheric turbulence and stability is manifested primarily in the description of vertical diffusion.

A detailed examination of the effect of variations in the vertical diffusion parameter (σ_z) is presented in Table 5. These values were selected from the extensive set of combinations of model inputs used in the general sensitivity analysis. They illustrate the complexity of the interrelationships of diffusion parameters with decay constant, wind speed and mixing ceiling. The most noticeable effect is the interaction between mixing ceiling and the diffusion parameter. Under a low mixing ceiling (100m) differences resulting from changes in σ_z are minimal, while under a high mixing ceiling (2500m) the diffusion parameter differences yield large differences in predicted concentrations.

Table 5. Model Concentrations with various Diffusion Functions for three Mixing Ceilings

a. When the Mixing Ceiling is 100m.

Input Parameters			Model Concentrations ($\mu g/m^3$) when the diffusion function is:		
Receptor Location	Half-Life	Wind Speed, m/sec.	Pasquill, Class E	McElroy-Pooler Class D	Class 1
Center	No Decay	2	1259	1207	1274
		6	547	402	425
		18	182	134	142
Center	30 min.	2	1146	819	850
		6	478	347	364
		18	174	127	134

b. When the Mixing Ceiling is 500m.(2)

Upwind	No Decay	2	12	3	2
Center		2	1635	703	520
Downwind		2	1526	440	525
Center	No Decay	6	545	234	173
	No Decay	18	182	78	58
	30 min.	6	476	214	158

c. When the Mixing Ceiling is 2500m(2).

Downwind	No Decay	2	1629	200	113
		6	543	67	38
		18	181	22	13
	5 min(1)	2	3	3	2
		6	4	2	1
		18	14	2	1

(1) A small sample of computer runs was made using a very large decay factor (5-min. half-life).

(2) Column headings in 5.b and c. as for 5.a.

5. REFERENCES

All references are included in Section 5. of the companion validation paper.

Chapter 27

COMPUTING OPTIMAL AIR POLLUTION ABATEMENT STRATEGIES

by

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on Air Pollution Modeling

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Computing optimal air pollution abatement strategies - some numerical experiments on field data.

by

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Abstract

The purpose of this paper is to present a method for calculating optimal air pollution abatement strategies applicable for multiple - source areas. In order to simplify the argument we shall consider only one single pollutant, although our analysis can be easily extended to the case when several different pollutants are studied simultaneously. We also confine the attention to the problem of long-term air pollution abatement, i.e. we discuss the monitoring of mean concentration taken over an extended period of time such as a month or the year. We shall assume that the sources can be split into several groups each of which can be regulated independently and that the contributions of the groups of sources combine according to the superposition principle. Using a diffusion model we construct for each group a function defining its contribution to the pollution. Hence it is possible to compute a regulatory strategy which meets given standards using available computer codes for linear and semi-infinite programming. However the output of most diffusion models consists of tables over irregular functions and these data are contaminated with large errors due to the fact that the physical processes involved are incompletely known. We therefore propose to smooth the tables using a least squares fit. Further we introduce preference functions defined in terms of physical entities such as population density and pollution concentrations. However,our proposed computational method is applicable for conventional economical preference functions also but costs are generally difficult to estimate. Our approach is tested on field data from Stockholm and the results are discussed in the last section.

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1. Preliminaries.

We treat the same general problem as in [Gustafson - Kortanek, 1973 a,b] . That is we consider an air pollution control area S, where several pollutors are present and the goal is to regulate the emissions in such a manner that an acceptable air quality is maintained while technical and administrative constraints are met and the impact costs are made as small as possible.

Acceptable air quality is defined by given standards which vary from country to country. See [Yanagisawa 1973] . Most countries have upper limits both for the time-average over shorter periods like 30 minutes (a short-term standard) and the average concentration over longer periods like a month or a year (long-term standards). We shall concentrate on the problem to meet a long-term standard for a single pollutant but our analysis can be directly extended to the case when standards for several pollutants must be met simultaneously. One may also consider both long-term and short-time standards at the same time.

We split the pollution sources into n groups each of which can be regulated independently. The contribution of group r is given by the transfer-function u_r, $r = 1,2,\ldots,n$. Further assume that the total concentration (averaged over time) given by χ and that the formula

$$\chi = \sum_{r=1}^{n} u_r \tag{1}$$

is valid. If now the emission from group r is reduced by the factor E_r then we shall assume that its contribution becomes

$$(1-E_r)\,u_r \tag{2}$$

and hence after regulation the concentration is changed from χ to χ_E where

$$\chi_E = \sum_{r=1}^{n} (1-E_r)\,u_r$$

Our goal is to select the reduction factors in such a manner that the given air quality standards are met. We note that E_r are constants and represent permanent reductions. Hence we shall not consider abatement strategies which call for temporary reductions under certain weather-conditions, nor shall we discuss the possibility to change the form of u_r e.g. by building higher stacks.

Often the subdivision of the pollutors into groups is suggested by the structure of the control problem at hand. Thus in the Chicago metropolitan area about 65 % of the sulphur oxides released into the air originates from 6 power plants [Roberts et al, 1970]. Therefore one might consider to split up the pollutors into 7 groups where the 6 first groups consist of one power plant each and the last group contains all the remaining pollutors. In other air pollution abatement problems some of the pollution comes from sources out-side the control area. Then it might not be possible to regulate them and their contribution must be taken into account as a back-ground pollution.

It is natural to seek an abatement policy which meets the air quality standard while minimizing the control costs incurred. Two difficulties hereby arize. First, control costs of many different kinds occur and it is not easy to describe them in a preference function. Second, an optimal policy might put a disproportionately heavy load on some pollutors while others get a better deal. These inequities might be remedied by means of a system of side payments. The questions mentioned in this paragraph are discussed in [Gorr - Gustafson - Kortanek, 1972].

Numerical determination of optimal control strategies on test problems using field data are reported by [Kohn, 1970].

In this paper we shall describe a case study for Stockholm. In Section 2 we describe the construction of the transfer functions u_r (concentration contribution) for a general case and in Section 3 we propose a preference function which is expressed by means of physical data only. Then in Section 4 we give an optimization model and the corresponding computational scheme and in Section 5 we discuss an application to Stockholm data.

2. Determination of the transfer functions.

Consider group number r of sources. If statistical data on wind speed, wind direction, stability class and mixing height together with a complete source inventory for group r is given then it is possible to determine a table over the concentration contribution u_r using a diffusion model See e.g.

[Fortak, 1970], [Gustafson - Kortanek, 1972], [Hanna, 1971] and [Bringfelt - Hjort - Ring, 1974]. The computed values of u_r are surely beset with errors, which may be systematic. The source inventory is incomplete and so is our knowledge of the transportation processes in the atmosphere. Further, the meteorological observations are not exact. Therefore we smooth the table of u_r in the following way.

1) u_r is tabulated at N points $x^1, x^2, \ldots x^N$

2) The total area of calculation S is divided into k subsets $S_1, S_2, \ldots S_k$

($k < N$) where S_j is selected as a rectangle if S_j is in the interior of S.

3) In each S_j we determine a linear function f_j^r

$$f_j^r(x) = a_j^r + b_j^r x_1 + c_j^r x_2 \text{, where } x = (x_1, x_2)$$

and the constants a_j^r, b_j^r and c_j^r are determined by the conditions a) and b) below

a) the function f^r given by

$$f^r(x) = f_j^r(x) \qquad x \in S_j$$

is continuous in the interior of S

b) The sum

$$\sum_{i=1}^{N} \left\{ \ln u_r(x^i) - f^r(x^i) \right\}^2$$

is rendered a minimum.

Our estimate for u_r will be $\tilde{u}_r$ when

$$\tilde{u}_r(x) = e^{f^r(x)}$$

Hence f^r is a linear spline which approximates $\ln u_r$ best in the least squares sense. It would seem more natural to approximate u_r instead of $\ln u_r$ but it turns out that then negative concentrations can be predicted.

One can prove the following results by means of straight-forward arguments if S is a convex set:

Lemma 1 Consider several different subdivisions of S in subsets S_j^ℓ of the type discussed above. Let $\tilde{u}_r^\ell$ be the corresponding estimate of u_r obtained as stated above. Denote by h^ℓ the longest side of any rectangle in subdivision ℓ. If u_r is a function with two continuous partial derivatives then there is a constant C depending only on u_r such that

$$\left|u_r(x) - \tilde{u}_r^\ell(x)\right| \leq C \cdot h_\ell^2 \quad \text{all } x \text{ in } S.$$

Lemma 2 Let $S_1, S_2, \ldots, S_k$ be a subdivision of S of the type defined above. Then $\tilde{u}_r$ is convex in each of the rectangular subsets of S.

Lemma 3 Let ρ_o be a given constant, $S_1, S_2, \ldots, S_k$ a subdivision of the type defined under 2) in this section. Estimate u_r with $\tilde{u}_r$ as described earlier. If $E_1, E_2, \ldots, E_n$ are such that:

$$0 \leq E_r \leq 1$$

and
$$\sum_{r=1}^{n} (1-E_r)\tilde{u}_r(x) \leq \rho_o \tag{3}$$

in each point x which is either an extreme point of S or a boundary point of S and belongs to two rectangles or lies in the interior of S and belongs to 4 rectangles then (3) holds in all of S.

The results mentioned in this section are illustrated in Figure 1.

S is split up into [illegible] rectangles $S_1, S_2, \ldots, S_{\text{[illegible]}}$. Hence 27 constants must be determined. We require continuity in the 12 points $A_1, A_2, \ldots, A_8$ and B_1, B_2, B_3, B_4 which gives 20 conditions on the coefficients. $\tilde{u}_r$ will be convex in each subrectangle and if (3) is met in the 16 A-, B- and C-points then it is fulfilled in all of S.

We note that if φ_o is the given standard, $\tilde{u}_r$ our estimates of the transfer functions then (3) is valid for all of S if it can be verified for the finite pointset given in Lemma 3. Further, Lemma 1 gives a bound for the systematic error we get when we replace u_r with $\tilde{u}_r$. This perturbation should be compared with the stochastical error.

The actual computation of $\tilde{u}_r$ once the table of $u_r(x^i)$, $i = 1,2,\ldots,N$ is known, can be carried out with the computer code given in [Björck, 1969]. However, one encounters large sparse matrices and therefore savings in storage and computation time can be achieved if more specialized codes are used.

3. Selection of preference function.

Let φ_o be the given standard. Then the abatement strategy defined by the numbers $E_1, E_2, \ldots, E_n$ is called admissable if

$$\sum_{r=1}^{n} (1-E_r)u_r(x) \leq \varphi_o(x), \quad x \in S$$

(In most applications φ_o is a constant but it is quite conceivable that $\varphi_o(x)$ might vary over S).

If there is an admissable vector E then there are generally infinitely many and the problem is to choose one which minimizes the drawbacks associated with forced emission reductions. This can be achieved by means of a cost-benefit analysis. See e.g. [Gorr - Gustafson - Kortanek, 1972]. However, very few attempts have been made to quantify costs (damages) and benefits. We mention here the study of regulating the emissions from steel industry, [Dunlap - Gorr - Massey, 1973].

Here we shall indicate how to derive a damage function which incorporates the effect of pollution on the people living in the air pollution control area S. We introduce the notations

χ_E is the concentration after reduction, described by the vector E

F is a given, nondecreasing function defined for a subset of the real axis

ω is a positive continuous function over the control area S

We define the total damage as the value of the functional D given by the integral

$$D(E) = \int_S \omega(x)\, F\,(\chi_E(x))dx$$

Compare Gorr, 1973 formula 2.2.7.)*

We illustrate with examples how various choices of ω and F correspond to different optimization policies.

1) **A standard defined by $\varphi(x) = \varphi_0$, $x \in S$ is given. No cost function is known.**

Then ω may be chosen arbitrarily (take e.g. $\omega(x) = 1$) and F is defined by

$$F(q) = \begin{cases} 0 & 0 \le q \le \varphi_0 \\ \infty & q > \varphi_0 \end{cases}$$

This means that a pollution policy is not admissable if χ_E reaches the value $1.01 \cdot \varphi_0$ in a small area even if $\chi_E(x)$ is far below φ_0 in the greater part of S. In contrast an abatement policy giving $0.98 \cdot \varphi_0 \le \chi_E(x) \le \varphi_0$ everywhere is "acceptable" and there is no incentive to do better. If only the industry's abatement costs are included an optimization will lead to an abatement policy which only considers the critical points and does not put a premium on improvements in areas where the standards are met already. The latters constitute the larger part of the area S.

2) F is linear function on $[0, \varphi_0]$. where φ_0 is a given constant standard. Then we define

$$F(q) = \begin{cases} q & 0 \le q \le \varphi_0 \\ \infty & q > \varphi_0 \end{cases}$$

Then we get if E defines an admissable policy

$$D(E) = \int_S \omega(x) \chi_E(x)dx = \sum_{r=1}^{n} (1-E_r)u_r$$

where

$$u_r = \int_S u_r(x)\omega(x)dx$$

Hence D is a linear functional in this case and the task to minimize D over all feasible E can be solved by means of existing codes [Fahlander, 1973], [Gustafson - Kortanek, 1973 a,b]. The quoted authors assume that E_r can vary continuously and this is often true in practice. If e.g. u_r represents emissions from houses one can introduce anti-pollution devices on any proportion of them.

The next question is the selection of ω. A natural choice is to make ω proportional to the population density. In the latest population census (of 1970) in Sweden the whole country was divided into small areas and the number of people in each was tabulated. Hence the local population density in 1970 can be accurately estimated. However, if a person spends only 12 hours at home each day and the remaining 12 hours elsewhere he should only be counted as 1/2 in the population tally of his neighbourhood. This refinement can be done since the number of people occupied in the different enterprises is known. Thus one can let $\omega(x)$ be proportional to the number of people-hours spent in the neighbourhood of x. We give an example of such a calculation in the last section.

3) F is progressively increasing over $[0, \varphi_s]$ where φ_s is the given standard. When F is linear and ω is defined as under 2) above the contribution to D(E) would be the same if 2 persons were exposed to a SO_2 concentration of 30 $\mu g/m^3$ as if 1 was exposed to 60 $\mu g/m^3$. It might seem more natural to assume that damage increases progressively with pollution. But then computational difficulties arise because D is not a convex function of E. We shall not treat this case here.

4. A general optimization model.

In this section we summarize our discussion and formulate our model in mathematical language. As earlier we consider an air pollution area S and assume that the pollutors have been split up into n groups whose contributions are represented by transfer functions $u_1, u_2, \ldots, u_n$. These are tabulated and the tables are smoothed as described in section 2 giving. $\tilde{u}_1, \tilde{u}_2, \ldots, \tilde{u}_n$. Each group can reduce its emission with a fraction E_r , $0 \le E_r \le e_r \le 1$ where e_r is a technical constraint. [illegible] standard is given. Further the economical costs of reducing emission is given by a function G which is continuous and convex (possible linear). We also assume that a budget B for pollution abatement costs is given and thus we get the constraint $G(E) \le B$. Hence we arrive at the optimization task:

Program I

Compute $C_B = \min D(E)$ for all vectors E subject to the constraints

$$\sum_{r=1}^{n} (1-E_r)\tilde{u}_r(x) \le \varphi_0 \qquad x \in S \tag{1}$$

$$0 \le E_r \le e_r \quad , \quad r = 1,2,\ldots,n \tag{2}$$

$$G(E) \le B \tag{3}$$

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As explained in Section 2 condition (4) may be replaced by finitely many linear constraints and hence Program I can be solved by means of conventional optimization codes. Several different outcomes are possible.

1) $$\max_{x \in S} \sum_{r=1}^{n} (1-e_r)u_r(x) > \varphi_0$$

Then the technical constraints (4) are too restrictive and must be reconsidered or one has to give up the ambition to meet the standard φ_0 .

2) $$\max_{x \in S} \sum_{r=1}^{n} (1-e_r)u_r(x) \le \varphi_0$$

Then there is a minimal budget $B = B_0$ such that the standard is met. Then we can solve Program I for various values of B and the change of the optimal value C_B gives the trade-off between the antipollution budget B and the value of the damage functional

Other questions might be analysed using program I. In the US two standards have been adopted: one primary to protect public health and one more stringen secondary which shall ensure public welfare. Let φ_0 and φ_1 ($\varphi_0 > \varphi_1$) be these two standards. One considers to implement the more stringent standard φ_1 and can do so with a certain antipollution budget B_1. However, if we keep the laxer standard φ_0 and use the same budget B_1, we get a lower optimal value of Program I. Hence we are faced with the choice between increasing the quality of the air in the worst polluted area and using the same resources for improving the overall quality as defined by D(E).

5. An application to Stockholm data.

We tested the methods presented in this paper on field data from Stockholm. The concentration of SO_2 in the air in metropolitan Stockholm is estimated by means of a model presented in [Bringfelt - Hjorth - Ring, 1974] . For illustration of the technique we use data for the month of February 1970 for a rectangular area 8.5 km by 6.5 km in the central part of Stockholm as shown in figure 2. The sources are divided into three groups (n = 3 in Program I):

(1) area sources (mainly space heating): u_1.

(2) temperature dependent sources (primarily centralized heating plants): u_2.

(3) process sources (temperature independent industrial emissions): u_3.

The contributions of these groups were calculated in a quadratic ($500 \times 500\ m^2$) grid with 221 gridpoints. The values given by the model are shown in Tables 1:1, 1:2 and 1:3. Hence these tables show the transfer functions u_1, u_2, u_3. Using least squares fit and requiring continuity as explained in Section 2 we get the smoothed transfer functions $\tilde{u}_1$ $\tilde{u}_2$ and $\tilde{u}_3$. The result of the smoothing is of course depending on how the subsets S_j are chosen. If we choose S_j large, then we might hope that the irregular errors will cancel out but according to Lemma 1 in Section 2 a systematic error is introduced. If S_j are small the local errors might result in unrepresentative values The best choice of S_j is a special problem for whose solution further study is necessary. In Tables 2 and 3 we give the result of smoothing u_1, the contribution from area sources taking S_j as squares $1.5 \times 1.5\ km^2$ and $2.0 \times 2.0\ km^2$ respectively.

Population data from the 1970 census were found in Nilsson - Vallas, 1972 They were used to estimate the number of people living in each square $500 \times 500\ m^2$. However, the areas whose populations are reported in the Census are irregularly shaped and since this is only a pilot study some simplifications were introduced.

Thus we assumed that the number of people-hours spent in each square was proportional to the number of persons reported as living there. Further, we only distinguished between the following categories of area for which average population densities are readily available: Water (a sizable portion of the area) 0 inh/km^2, central Stockholm 7934 inh/km^2, Southern suburbs (Söderort), 3875 inh/km^2, Western suburbs (Västerort), 2262 inh/km^2, Solna 2489 inh/km^2 and Lidingö 1193 inh/km^2. For each square then the percentage of the area which belongs to the categories mentioned above was assessed from a map and its population was estimated as a weighted average. From this simple calculation Table 4 emerged. No data could be found for the cost of abatement but since our purpose is to test our computational scheme we choose arbitrarily $G(E) = 10E_1 + E_2 + 3E_3$ in the budget constraint (6) with $B = 9$. The technical constraints were taken to $e_1 = 0.8$, $e_2 = 0.9$, $e_3 = 0.8$ and the standard $\varphi_o = 80\ \mu g/m^3$ was assumed. The results are given in Table 5.

Conclusions.

Optimal air pollution abatement policies can be computed using existing computer codes for least square fitting and linear programming. The computational effort for optimization is negligible in comparison to the cost of constructing the transfer functions which are needed for any prediction of concentration of pollutants. The additional computing cost of optimization might be further reduced if sparse matrix techniques are used. The error caused by the discretization, that is the representation of the control area by a finite grid might be estimated using the theory of semi-infinite programming, [Gustafson - Kortanek, 1973 a] . The selection of air quality standards and preference function reflects the value scale of the decision maker and is hence a political issue since all the members of the society cannot be expected to have the same preferences. Hence bargaining between interest groups can occur. Optimization models makes it possible to explore the effects of various choices of preference function, air quality standards and anti-pollution budgets.

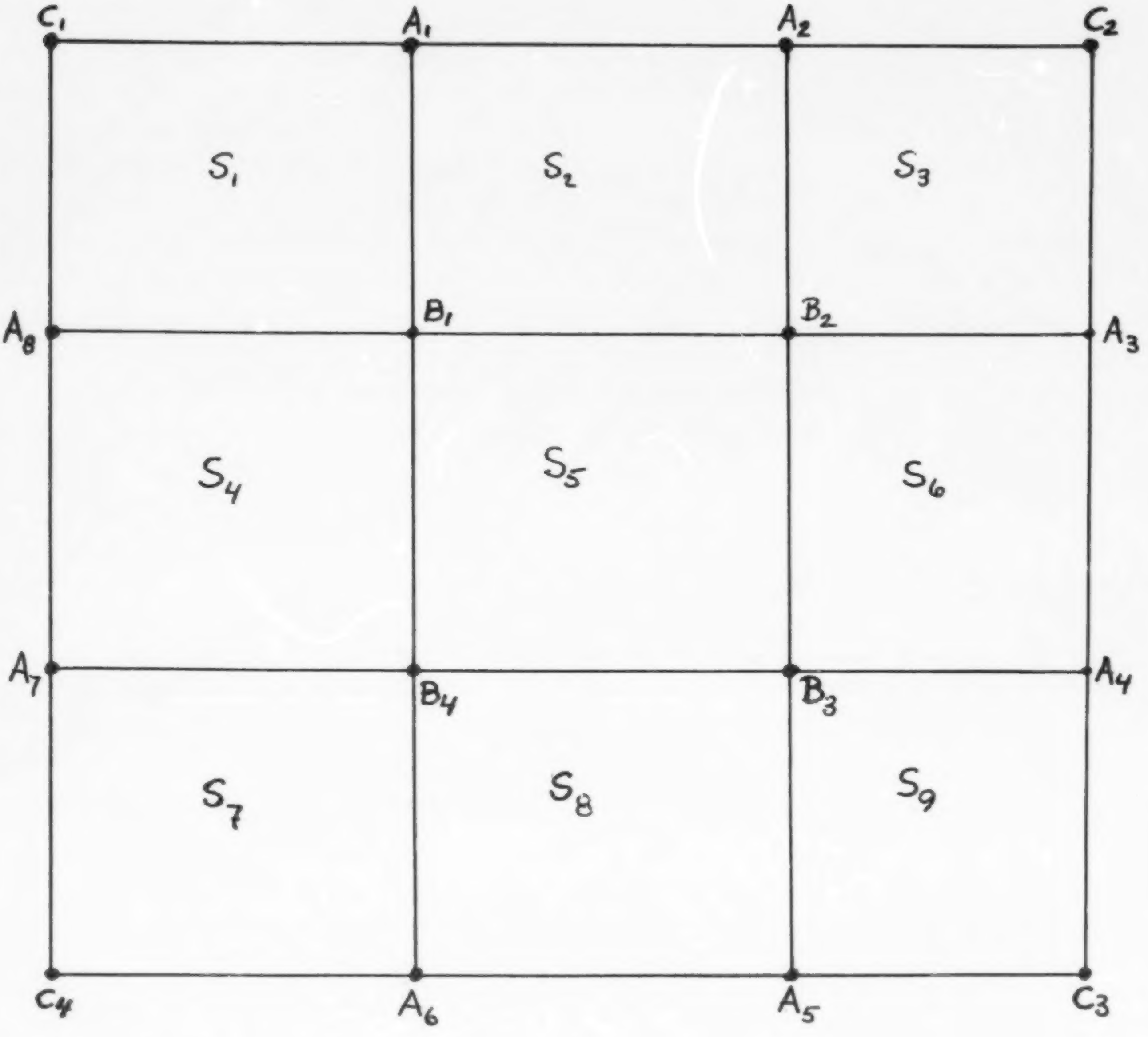

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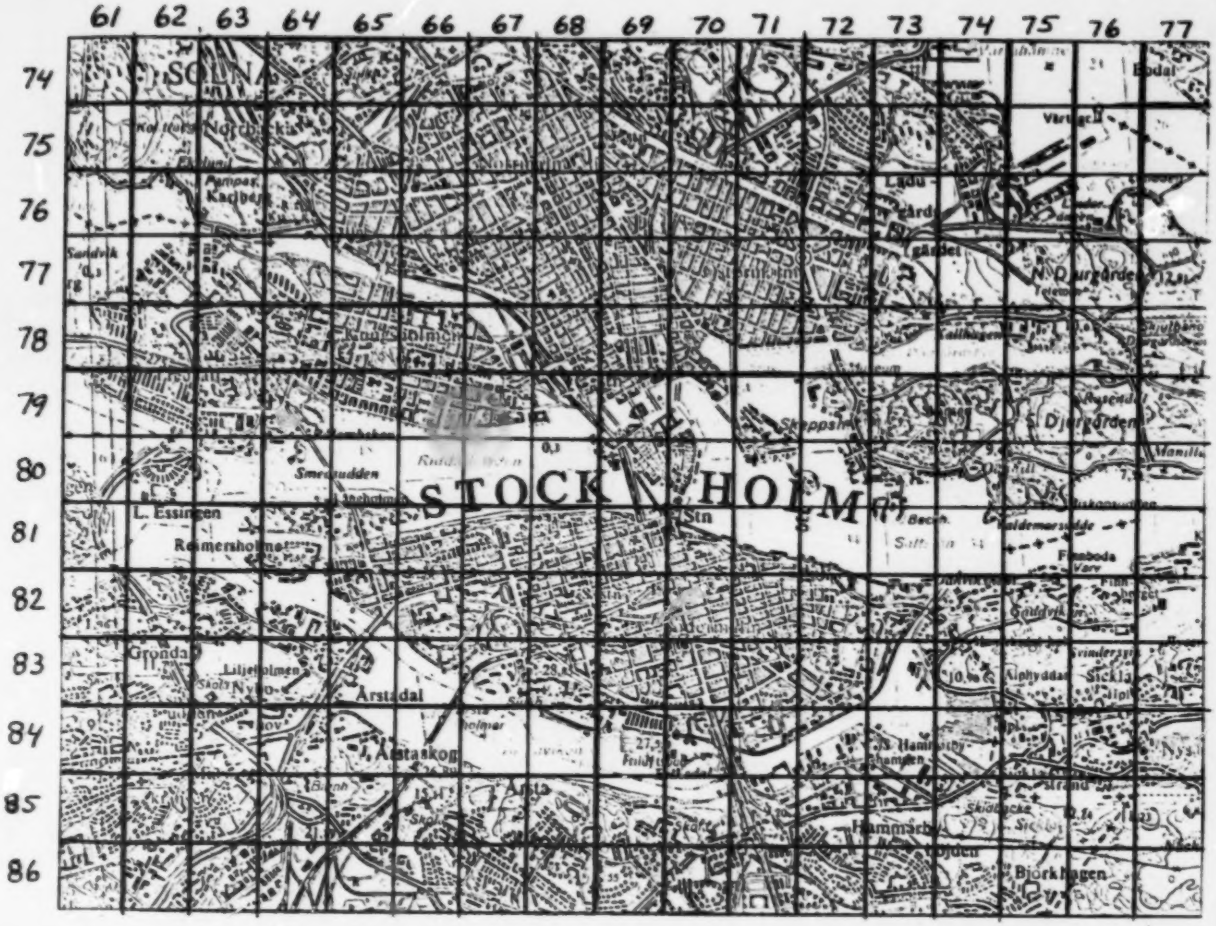
Figure 1. For explanation see text.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Reimersholme
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Årstadal
Skeppsh
S. Djurgården
N. Djurgården
Hammarby
Björkhagen

Figure 2. 500 x 500 m^2 grid system used. The numbers refer to the coordinate-system used.

	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77
74	151	150	147	150	164	196	220	234	228	215	205	199	190	182	170	162	158
75	154	151	152	163	199	263	301	328	321	291	273	260	238	221	202	186	175
76	165	162	166	188	251	304	337	377	384	362	343	316	275	244	219	201	187
77	188	196	201	220	276	295	321	374	409	416	401	355	305	264	232	211	195
78	196	195	200	219	276	293	301	334	385	380	377	343	295	254	226	207	191
79	184	194	201	214	258	285	299	302	312	319	308	286	260	236	216	201	189
80	193	200	200	204	226	241	253	266	287	298	291	269	248	230	214	201	196
81	205	213	208	207	235	254	265	294	326	337	321	291	259	236	221	208	198
82	208	238	248	239	255	260	260	290	315	336	348	328	286	253	231	217	206
83	225	248	251	240	239	237	244	268	294	324	341	322	281	252	234	226	214
84	240	258	254	243	236	234	241	255	273	290	295	285	264	244	233	226	213
85	270	281	280	268	252	252	270	266	297	302	298	293	276	258	254	244	222
86	252	248	253	253	247	256	276	294	304	305	304	308	297	284	273	246	219

Table 1:1 Contributions from area sources to average concentration for Feb 1970 as predicted by the diffusion model ($\mu g/m^3$).

	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77
74	2	2	3	3	3	3	3	3	3	3	3	2	3	2	3	4	5
75	3	3	3	3	3	3	4	4	3	4	4	4	4	4	4	4	4
76	2	3	3	4	3	3	4	4	4	4	4	4	5	4	4	4	4
77	2	2	4	3	4	4	5	4	5	5	5	6	6	6	6	5	5
78	2	3	3	3	3	3	4	4	4	4	4	5	5	5	5	4	4
79	2	3	3	3	3	3	3	4	3	3	5	7	6	7	5	4	4
80	3	2	2	2	2	3	4	3	4	5	5	6	5	5	5	4	4
81	3	2	2	2	3	3	3	4	5	4	4	6	5	4	4	3	3
82	2	2	2	2	2	3	3	4	3	5	5	4	4	3	4	3	4
83	2	2	2	2	3	3	4	4	4	4	5	4	4	3	4	3	5
84	2	2	3	3	3	3	4	4	5	4	5	3	5	3	4	3	5
85	1	2	3	3	3	4	4	3	4	3	6	3	4	3	5	4	4
86	2	3	3	3	4	3	4	3	3	2	4	3	5	3	4	4	4

Table 1:2 Contributions from process sources (temperature independent) to average concentration for Feb 1970 as predicted by the diffusion model ($\mu g/m^3$).

	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77
74	23	23	24	23	23	25	27	32	27	37	41	36	31	29	31	29	31
75	23	25	26	27	27	28	28	29	31	33	40	40	38	37	35	39	32
76	22	25	27	27	29	31	30	31	46	37	35	39	37	40	34	31	35
77	20	23	31	29	32	33	34	34	43	43	47	40	39	45	38	39	37
78	20	24	25	26	30	33	34	41	46	51	46	44	42	41	40	43	36
79	21	29	28	28	29	30	34	42	42	49	45	45	42	38	42	35	37
80	18	23	25	25	30	32	38	42	42	42	48	40	39	38	35	38	32
81	18	21	24	26	27	31	40	47	43	48	39	40	45	39	40	35	37
82	18	21	22	25	28	30	38	45	42	39	42	39	40	41	39	46	39
83	19	21	23	26	27	33	37	42	40	39	41	38	37	41	38	38	37
84	22	23	25	27	30	35	37	39	40	37	40	37	38	37	43	35	39
85	20	23	26	27	40	35	39	38	39	35	38	33	43	36	42	37	35
86	21	26	28	29	34	33	40	37	36	32	35	33	36	33	35	39	32

Table 1:3 Contributions from temperature dependent sources to average concentration for Feb 1970 as predicted by the diffusion model (μg/m^3).

	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77
74	155	157	159	167	181	197	212	228	244	246	233	221	206	190	175	161	148
75	173	176	178	187	203	221	238	252	274	276	262	248	232	213	196	181	166
76	194	197	200	210	228	248	267	286	307	310	293	278	260	239	220	202	186
77	218	221	224	235	256	278	300	321	345	347	329	312	291	268	247	227	209
78	223	227	230	241	262	285	307	329	353	356	337	320	298	275	253	233	214
79	209	213	216	226	246	267	288	309	331	334	316	300	280	258	237	218	201
80	196	199	202	212	230	250	270	290	311	313	297	281	262	241	222	205	188
81	194	197	200	210	227	247	266	286	307	309	293	277	259	238	219	202	186
82	201	204	207	218	236	257	277	297	319	321	304	288	269	248	228	210	193
83	209	212	216	226	246	267	288	309	331	334	316	300	280	257	237	218	201
84	214	218	221	232	252	273	295	316	339	342	324	307	287	264	243	223	206
85	217	220	223	234	254	276	298	319	343	345	327	310	289	266	245	226	208
86	219	222	225	236	257	279	301	323	346	349	330	313	292	269	248	228	210

Table 2. Area sources: Results after smoothing, taking S_j as squares 1.5 x 1.5 km^2.

	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77
74	162	167	172	178	189	208	228	251	259	251	244	237	223	204	187	171	156
75	173	178	184	189	201	221	243	267	276	268	260	252	237	217	199	182	167
76	184	190	196	202	215	236	259	285	294	285	277	268	253	232	212	194	178
77	196	224	209	215	229	251	276	303	313	304	295	286	270	247	226	207	189
78	209	216	222	229	244	268	294	323	334	324	314	305	287	263	241	220	202
79	214	220	227	234	249	273	300	330	341	331	321	311	293	268	246	225	206
80	209	215	222	229	243	267	294	323	333	323	314	304	287	262	240	220	201
81	204	211	217	224	238	261	287	316	326	316	307	298	280	257	235	215	197
82	200	206	212	219	233	256	281	309	319	309	300	291	274	251	230	210	192
83	200	207	213	219	233	257	282	310	320	310	301	292	275	252	281	211	193
84	206	213	219	226	240	264	290	319	329	319	310	301	283	259	237	217	199
85	213	219	226	233	247	272	299	328	339	329	319	309	292	267	244	224	205
86	219	225	232	239	255	280	308	338	349	339	328	319	300	275	252	230	211

Table 3. Area sources. Results after smoothing, taking S_j as squares 2.0 x 2.0 km^2.

	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77
74	2.8	2.8	2.8	2.8	3.9	2.9	7.9	7.9	7.9	7.9	7.9	7.9	7.1	5.6	0	0.2	0.8
75	2.8	2.8	2.8	2.8	7.4	6.4	7.9	7.9	7.9	7.9	7.9	7.9	7.9	7.1	1.6	1.6	0.1
76	0.3	1.4	3.0	4.9	7.9	7.9	7.9	7.9	7.9	7.9	7.9	7.9	7.9	7.9	7.1	7.1	3.2
77	3.4	7.9	3.9	7.9	7.9	7.9	7.9	7.9	7.9	7.9	7.9	7.9	7.9	7.9	7.9	7.9	7.9
78	7.1	7.9	3.9	7.9	7.9	7.9	7.9	7.9	7.9	6.4	6.4	6.4	4.8	3.2	6.4	7.1	7.9
79	3.2	7.1	3.9	7.1	5.6	7.1	6.4	5.6	7.1	1.6	1.6	6.4	6.4	7.9	7.9	7.9	7.9
80	3.2	5.6	1.6	1.6	1.6	0	0	0.8	6.4	1.6	1.6	2.4	6.4	7.1	7.1	5.6	4.2
81	0.8	0.4	2.4	7.9	7.9	6.4	7.1	7.1	7.1	5.6	1.6	0.8	0.8	0.8	0.8	0	1.6
82	3.5	3.9	6.8	3.5	5.6	7.9	7.9	7.9	7.9	7.9	7.9	7.9	7.1	3.1	3.5	3.5	1.2
83	3.9	3.5	1.9	3.9	1.6	3.2	7.1	7.9	7.9	7.9	7.9	7.1	3.1	3.9	3.1	3.1	3.5
84	3.9	3.9	3.9	3.9	3.1	0.8	0.8	2.4	6.4	6.4	7.1	4.7	2.3	3.9	3.9	3.9	2.7
85	3.9	3.9	3.9	3.9	3.9	3.9	3.5	3.1	2.7	2.7	3.9	3.9	3.9	3.9	3.9	3.9	3.9
86	3.9	3.9	3.9	3.9	3.9	3.9	3.9	3.9	3.9	3.9	3.9	3.9	3.9	3.9	3.9	3.9	3.9

Table 4. Estimated population density in the squares of the grid (thousands of inhabitants per km^2)

Table 5

Experimental computation of optimal abatement policy for central Stockholm based on data for Febr. 1970.

$\varphi_0 = 80\ \mu g/m^3$ $n = 3$

$e_1 = 0.9$ $e_2 = 0.9$ $e_3 = 0.8$,

$\mu_1 = 291565$ $\mu_2 = 38322$ $\mu_3 = 4122$

$10E_1 + E_2 + 3E_3 \leq B$

Solution: E_1^*, E_2^*, E_3^*

Optimal value: $C_B = \sum_{r=1}^{3} \mu_r(1-E_r^*)$

1) $S_j = 1.5 \times 1.5\ km^2$ $B = 9$ infeasible

2) $S_j = 1.5 \times 1.5\ km^2$ $B = 10$ $E_1^* = 0.9$ $E_2^* = 0.9$ $E_3^* = 0.033$
$C_B = 3.697 \cdot 10^4$

3) $S_j = 2.0 \times 2.0\ km^2$ $B = 9$ $E_1^* = 0.8$ $E_2^* = 0.9$ $E_3^* = 0.033$
$C_B = 6.613 \cdot 10^4$

4) $S_j = 2.5 \times 2.5\ km^2$ $B = 9$ $E_1^* = 0.8$ $E_2^* = 0.9$ $E_3^* = 0.033$
$C_B = 6.613 \cdot 10^4$

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Chapter 28

MODELING FOR SUPPLEMENTARY CONTROL SYSTEMS

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
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PRESENTED AT THE 5th MEETING OF NATO/CCMS
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1. INTRODUCTION

Supplementary control systems (SCS) are systems whereby the rate of emissions from a given pollutant source are reduced by emissions reductions or control on the basis of observed or forecasted adverse meteorological conditions. Thus, under conditions of poor atmospheric dispersion, an emissions reduction is called for (say by switching to a lower sulfur content fuel) to avoid the occurrence of high ground-level concentrations.

Because of the very great expense and obvious non-optimum nature of simple, across-the-board rollback procedures for sulfur emissions, there is growing desire within the power industry and other concerned and competitive industries to optimize the use of fuels for minimum cost with the constraint that air contamination be maintained below all applicable ambient standards. It is argued that as long as air quality is maintained at concentration levels below those required by the most stringent standard, then the method which promises lowest total costs should be utilized. Clearly, the enforcement of simplistic rollback and absolute emissions limits does not allow for any sophisticated system to jointly optimize costs and environmental impact. The concept of the SCS, however, can be aimed exactly at that optimization.

A major question regarding the use of SCS systems is the expected reliability of these systems with respect to maintaining air quality standards. ERT's study (Reference 1) performed for the U.S. Environmental Protection Agency (EPA) presents a methodology for evaluating the reliability of SCS systems in terms of probabilities of exceeding air quality standards as a function of emission factors, meteorological conditions, and control strategy.

2. BACKGROUND INFORMATION ON SUPPLEMENTARY CONTROL SYSTEMS

2.1 Types of Supplementary Control Systems

For power-generating stations and industrial processes, there are three types of supplementary emission controls which can be adopted: fuel switching, load shifting, and process curtailment. The general aspects of these control measures are summarized below.

Fuel Switching involves the use of two or more fuels, with different sulfur content, according to a plan designed to meet specific air pollution control criteria. Because the fuels are usually differentiated with respect to sulfur content they have different impacts on air quality. At present, the principal control method for SO_2 and SO_3 emissions is the use of low sulfur fuels. An example of fuel switching would be a facility using 2% or greater sulfur content fuel during times when local ventilation is good, switching to 0.5% sulfur content fuel during times of poor dispersion. This type of control results in a negligible reduction in plant production.

In practice, three time scales for fuel switching have been proposed for individual facilities:

1. Normal operational use. This would constitute short period switching in which a facility would be operated with switching on a daily basis, or more frequently if desired.

2. Seasonal use. Because SO_2 emissions related to space heating demands do not occur in the summer months, power-generating facilities might use a higher sulfur content fuel during these times, saving the low sulfur fuel for use in the winter period.

3. Emergency use. A power-generating station might operate with a limited reserve of low sulfur fuel, for use during a few days of each year, when specific local pollution problems occur.

Fuel switching operations with oil are relatively simple compared with switching between high and low sulfur coal. The coal switch requires not only extra storage and handling facilities, but possibly two feed bunkers instead of one;and a time delay of several hours could occur before changes in SO_2 emission levels would be apparent in the stack.

Load Shifting involves the controlled operation of two or more generating stations which are interconnected by power transmission lines, and under the control of a common dispatch center. Load shifting for air quality control is accomplished when the dispatching practices developed for a group of stations are modified to incorporate consideration of the total regional impact of the interconnected stations. In addition to load shifting program, fuel switching can be simultaneously practiced at individual stations within a network.

Load shifting for air pollution control purposes is possible only when an interconnected group of generating stations has capacity in excess of demand. Many of the power networks within the United States operate near capacity at certain times of the day and year. However, almost all networks have excess capacity some of the time; for example, during the late night-early morning period (typically, from 10 PM to 6 AM local time).

Shepard (1970) has performed a case study analysis of a proposed load shifting plan for the generating stations in the St. Louis area. He found that significant reductions of population exposures to SO_2 are possible with small increases (about 5%) in power-generating costs for the region. Shepard's analysis treated only load shifting operations, without consideration of fuel switching at single stations. Because of the current price differentials between fuels with various sulfur contents, fuel switching operations can result in even greater cost efficiencies than those cited by Shepard for the load shifting case.

Curtailment of an industrial process is a conceptually simple way to achieve dynamic emission controls, and sometimes the most practical. When air quality standards are violated some small fraction of the total time, significant emissions reduction can be achieved by cutting back operations when standards are threatened.

Other possible types of supplementary control methods include dynamic controls of stack gas temperatures to enhance plume rise or intermittant use of scrubbers or similar emission cleaning devices during adverse meteorological conditions.

2.2 Current Supplementary Control Systems

Tennessee Valley Authority

Load shifting is being demonstrated by the Tennessee Valley Authority (TVA, 1973) as a feasible, reliable form of dynamic emissions control for meeting air quality standards. In September 1969, TVA began operating an SO_2 limitation program at their Paradise Steam Plant in west-central Kentucky.

Plant-generating load reductions reduce emissions whenever plume dispersion is unfavorable. These conditions are identified by on-site meteorological measurements which measure adverse atmospheric dispersion characteristics. The TVA program includes extensive pre-operational field studies to monitor maximum ground-level concentrations and collect added information about plume characteristics through helicopter and mobile ground measurements. This information is combined with output from a critical plume dispersion model to establish nine meteorological and plume dispersion criteria to determine when critical conditions threaten standards and require emissions reductions.

American Smelting and Refining Company

The American Smelting and Refining Company (ASARCO) has demonstrated the effectiveness of a program for emissions control by curtailing smelter operations. ASARCO has installed a control system that includes 18 SO_2 monitoring stations at their El Paso smelting complex. The system enables ASARCO to curtain operations to reduce or eliminate unacceptable SO_2 concentrations. A real-time method of monitoring and forecasting concentrations has been developed to enable ASARCO to achieve earlier, preventive curtailment and further reduce the time lag between detection and reversal of an upward trend in SO_2 concentrations. ASARCO curtailment programs for dynamic emissions control at their El Paso and Tacoma complexes have substantially reduced their air quality violations.

Environmental Research & Technology, Inc.

Environmental Research & Technology, Inc. (ERT), has been operating a real-time SO_2 monitoring and forecast system in Massachusetts and New York State since December 1971. This system is called AIRMAP^R, an acronym which stands for Air Monitoring Analysis and Prediction. AIRMAP operations and data over more than 24 months demonstrate the feasibility and reliability of optimizing air quality through dynamic emissions control in the Boston area.

The AIRMAP program consists of field sensors, telemetry, analysis software, and prediction techniques to monitor and predict ambient air quality and monitor stack emissions. It is an integrated software-hardware system. Data is reported back from the sites to the AIRMAP Centrals once every minute via dedicated telephone lines. The prediction component of the system, which has proved to be highly accurate, provides forecasts of air quality a day in advance. These forecasts form an integral part of the dynamic emission control procedures.

The AIRMAP system will soon include more than 200 monitoring sites measuring a total of more than 900 parameters (SO_2, NO_2, NO_X, coefficient of haze, wind direction and wind speed, temperature, etc.)

2.3 U.S. Federal Regulations Regarding Supplementary Emission Control

On 31 May 1975, air quality throughout the United States must meet primary ambient air quality standards for a series of pollutants. The Clean Air Act and Amendments thereto establish national primary ambient air quality standards to protect public health. These standards specify limits on ground-level concentrations of various pollutants including sulfur dioxide (SO_2).

Recently the EPA proposed additional regulations for the use of SCS systems for a small number of large isolated sources. The proposed regulations impose stringent limitations on the types of sources and situations for which use of SCS may be considered acceptable.

The two principal considerations in determining SCS acceptability are:

- The system must be only a supplement to the best available constant emission controls. This restriction implies that the source must actively investigate emission control technology and must implement new control techniques as they become available.
- The system must exhibit a high degree of reliability and must be made legally enforceable.

Our work addresses the latter consideration for SCS acceptability. Some important elements of the proposed regulations relevant to the reliability of SCS systems are included below:

- The SCS must have an SO_2 monitoring network with an array of sampling points located where maximum ground-level concentrations are most likely to occur. The number of monitors must also be sufficient to calibrate a model for interpolation between monitors.

- The SCS must have an operating model which relates meteorological inputs, emission rates, source data, terrain, and location factors to ambient air quality.

- The SCS must have meteorological parameter observations and prediction for use in air quality forecasts. Similarly, the source must have continuous emissions monitoring and forecasting.

- Objective rules for emission control must exist. These rules relate air quality predictions to a controlled emissions schedule.

- The SCS source must conduct a comprehensive background study of not less than 120 days. The results of this study must, among other requirements, provide objective reliability tests to measure the ability of the SCS to protect against violations of national standards.

- The source must define a program whereby they systematically evaluate and improve the reliability of the supplementary control system.

The above list of SCS requirements will force a degree of uniformity among acceptable SCS plants. The reliability analysis methods developed in the next sections are adaptable to any SCS which satisfies the EPA guidelines.

3. RELIABILITY ASSESSMENT

3.1 Definition of Reliability

Throughout this article the reliability of an SCS will be expressed in terms of the probability of violation of air quality standards anywhere within the region of influence of the controlled source. The time scale of the reliability estimates are determined by the form of many of the air quality standards which require violations "not to be exceeded more than once per year".

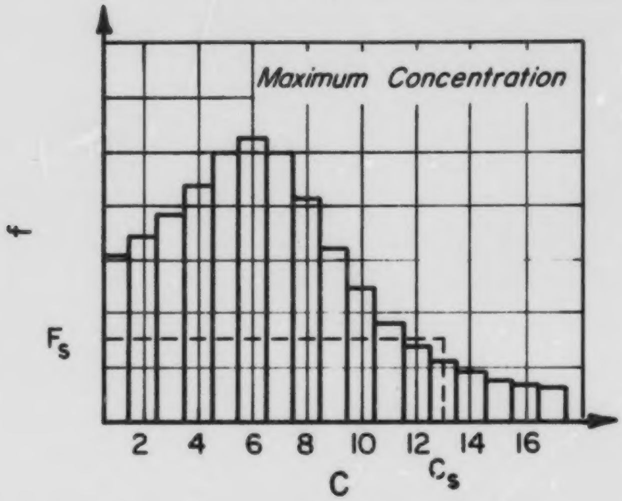
The specification that an air quality standard not be violated "more than once per year" has been interpreted in this work in probabilistic terms to require that the projected frequency of occurrence of violations of that standard be less than once per year. This probabilistic interpretation is necessary to develop quantitative analysis of reliability.

3.2 Probability Concepts Relevant to an SCS Analysis

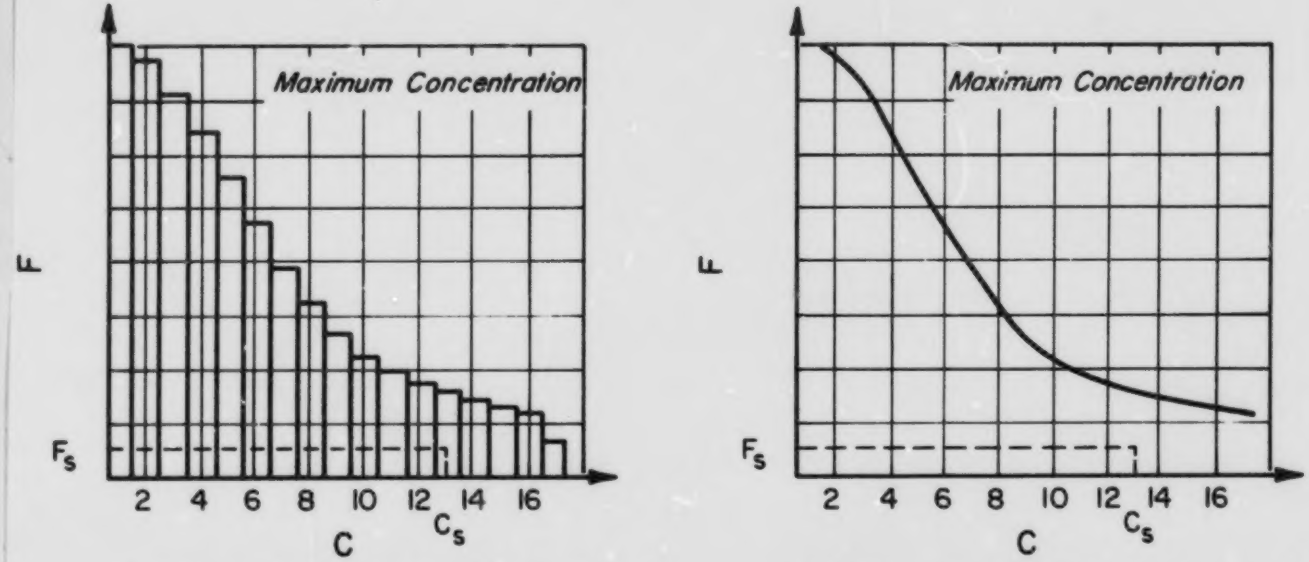
Figure 1 illustrates typical frequency distributions of air quality levels from point sources whose contributions dominate the concentration fields. The top figure is representative of a distribution of highest concentrations at any one of a network of receptors around a source.

The value C_s has been designated on the abscissa of the maximum concentration graph to indicate the value of some air quality standard. The sum of the frequencies of occurrence of all concentration categories greater than C_s is the fraction of the time the air quality standard is expected to be exceeded. The value F_s on the ordinate of each graph has been designated to indicate the permissible frequency of concentration values exceeding C_s. To satisfy air quality standard the sum of the frequencies for values of concentration to the right of C_s must be less than F_s. Thus, from a compliance view point, the more useful distribution is the cumulative frequency distribution (middle figure) associated with the frequency distribution discussed above. In this case, the sum of the frequencies of all values greater than the abscissa value is plotted as the ordinate. The sum over the frequency distribution of occurrence for concentrations greater than C_s can now be read directly from the ordinate of the graph.

For analysis purposes, the step function presentation of the cumulative frequency distribution can be replaced by a smooth function as illustrated



a) Discrete Frequency Distribution



b) Discrete Cumulative Frequency Distribution

c) Continuous Cumulative Frequency Distribution

Figure 1 Representative Frequency Distributions for the Maximum Ambient Concentrations from a Point Source.

in Figure 1(c). Using the graphs of Figure 1(c), it can be simply stated that the goal of any control procedure is to reduce the locus of F at the abscissa value C_s below the dashed line representing F_s.

The cumulative frequency distribution can be used to illustrate the effects of any control procedure. Figure 2(a) shows a hypothetical distribution of maximum ground level concentrations. Since the locus of the uncontrolled F is above the dashed line at $C = C_s$, the source is in violation of standards. Direct application of a constant emission control which reduces emissions uniformly by 50% (say, changing from 2% to 1% sulfur fuel or installing 50% efficient removal devices) would move every value of F from the abscissa value C to the abscissa value C/2 to yield the controlled F* curve illustrated. The graph of F has been reduced, as required, below F_s to satisfy the air quality requirements. More generally, we could have effectively moved every value of F from C to $\beta \cdot C$ where β is any value less than β_o such that $F(C_s/\beta_o) \leq F_s$. The resulting value of $F^*(C) = F(c/\beta)$.

An alternative to a rigid emission control system such as discussed above would be an SCS capable of changing the tail of the graph to F to reduce F* to values below F_s for $C \geq C_s$.

Figure 2(b) represents a frequency distribution resulting from the operation of an SCS. The curve of F* is not different from the curve of F at the low concentration end of the graph. This is in contrast to the constant emission reduction case of Figure 2(a) where all concentrations (even those well below standards before controls) are reduced. The tail of the F* curve of Figure 2(b) is below the dashed line for values of $C > C_s$ as required. The values of $C > C_s$ would be the result of uncertainty (errors) in the operation of the SCS, but their expected frequency of occurrence is so low that a reliable SCS is still maintained.

The analysis of SCS systems which follows is based upon consideration of modifications to the frequency distributions as discussed above.

3.3 Design of an Analysis Scheme to Measure the Reliability of a Supplementary Control System

3.3.1 Assumptions and Definitions

A computer program PROBL has been developed to generate the frequency distribution of maximum ground-level concentrations due to the source under

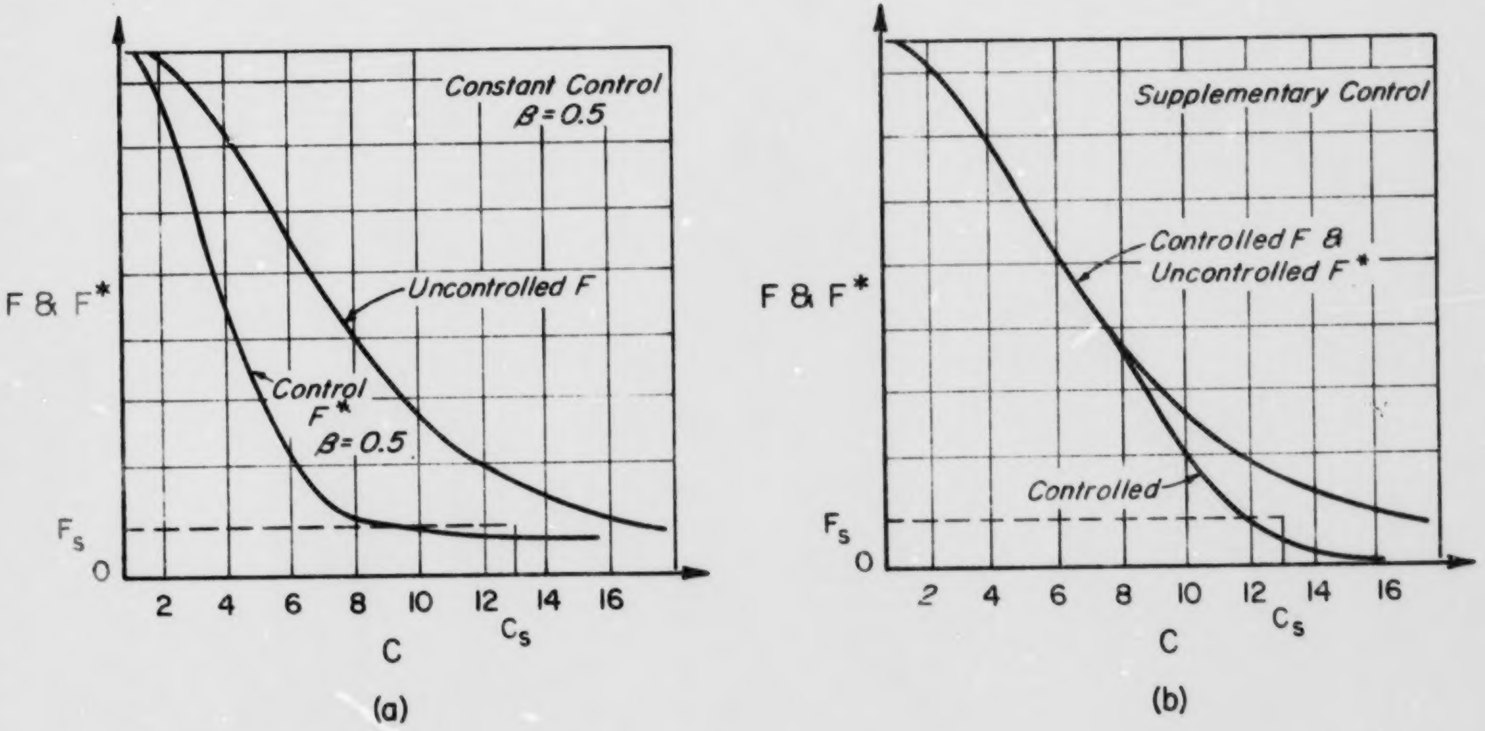


Figure 2 Representative Cumulative Frequency Distributions for Maximum Concentrations under Conditions of: a) No emission controls and constant emission reduction, b) supplementary emission controls.

study with or without emission controls. In particular, the program can generate the frequency distribution for a wide variety of possible SCS schemes.

The main assumptions of the analysis scheme are the following:

- A single source of SO_2 is responsible for observed concentration levels;
- Without an SCS, emissions are independent of meteorological conditions;
- With an SCS, emissions are controlled according to rules which depend on predicted meteorological conditions;
- Errors in meteorological predictions are independent of meteorological conditions. (This assumption can be relaxed).

To describe the model, we first define the following:

$c(x,t)$: concentration at time t and location x
$C(t)$: max $c(\underline{x},t)$; maximum concentration over all x locations at time t
$\underline{x}$: downwind location of $C(t)$
C_s: air quality standard or SCS threshold
$Q(t)$: emission rate without SCS
$M(t)$: meteorological function relating the maximum concentration $C(t)$ to source emission rate $Q(t)$ which will include the effects of stack height, wind conditions, mixing depths or any other pertinent meteorological inputs
$R(t)$: the error ratio of concentration prediction defined as follows:

With or without an operating SCS, the observed maximum concentration C_o is related to the actual emission rate Q through the meteorological function M as follows:

$$C_o = Q \cdot M \text{ at time } t$$

With an operating SCS, the corresponding maximum predicted concentration is related to the actual emission rate Q and the meteorological function M (defined above) through the Error Ratio R as follows:

$$C_p = Q \cdot M \cdot R \text{ at time } t$$

From the above, the error ratio can be defined as

$$R = C_p/C_o$$

The observed maximum concentration under SCS control is given by $C_c = Q_c \cdot M$ where Q_c is the SCS controlled emission rate determined from the forecast concentration C_p.

The value of Q_c depends on the SCS control strategy being used. Two examples of possible control strategies are:

1) Fuel Switching

$$Q_c = \begin{cases} Q & \text{if } C_p < \gamma \\ \beta Q & \text{if } C_p > \gamma \end{cases} \qquad \text{(Strategy 1)}$$

where β is a constant (less than one) which depends on the nature of the fuels. A switch from 2% sulfur fuel to 0.5% sulfur fuel means $\beta = 0.25$ The threshold parameter γ is a function of the air quality levels attempted to be maintained.

2) Process Curtailment

$$Q_c = \begin{cases} Q & \text{if } C_p < \gamma \\ \gamma/C_p \cdot Q & \text{if } C_p > \gamma \end{cases} \qquad \text{(Strategy 2)}$$

In general, the threshold γ needs to be set below standards to provide a margin of safety. Q(t) can be a well defined quantity if emission monitors are used or if emission rate is simply related to the production rate or to the load of the plant under study. If the plant emissions are not monitored some engineering estimates of the frequency distribution of Q can often be made from production or process control information.

The function M(t) can be determined in various ways. For an operation with an extended historical air quality monitoring record, M(t) could be estimated from the ratios of measured maximum concentrations $C_o(t)$ and known emission rates Q(t). Alternatively, where little site monitoring data exists, outputs from any type of air pollution model can be used in conjunction with historical meteorological data to construct M.

The function R(t) may be determined from historical real-time monitoring and forecasting data. Since the function R will depend upon the unique forecasting difficulties for each SCS scheme, initial estimates of R must be evaluated during the design and initial testing of the SCS. The upgrading of an SCS as time proceeds will involve periodic re-evaluations of this function.

Given the functions Q(t), M(t) and R(t) over an appropriate averaging time period, frequency of occurrence distributions can be readily derived for the various magnitudes of the observed or determined values of Q, M and R. Thus, the time history data is transformed into a frequency of occurrence distribution. For purposes of future estimations, the frequency of occurence distributions become expected probability density functions.

When the frequency distributions for Q, M and R as defined above are determined, the analysis scheme is capable of generating the following basic information.

1. The number of violations to be expected without and with any SCS scheme.

2. The percentage of production lost if the SCS scheme is a load reduction program.

3. The percentage use of high and low sulfur fuel in a fuel switching SCS program.

4. The dependence of the number of violations, production lost and/or percentage use of high and low sulfur fuel upon the implementation threshold (γ), model calibration, meteorological forecasting skill, and/or the difference in sulfur content of the two switching fuels.

The mathematical description of the PROBL model is given below.

3.3.2 The Mathematical Description of the SCS Analysis Scheme

Define P_X as the probability density function for the variable X. Then the probability of the variable X having a value between a and b is

$$F_X = \int_a^b P_X(\zeta)\, d\zeta$$

Assume that there exist probability density functions for M and Q, and we wish to generate a frequency distribution for C when no SCS is operating. If A is any concentration value, ε is a variable and Q and M are independent of each other and random variables, then

$$\begin{aligned} P_C(C = A) = \Big[& P_Q\,(Q = \varepsilon) \cdot P_M\,(M = A/\varepsilon) + \\ & + P_Q\,(Q = 2\varepsilon) \cdot P_M\,((M = A/2\varepsilon) + \text{---} \\ & + P_Q\,(Q = n\varepsilon) \cdot P_M\,(M = A/n\varepsilon) + \text{---} \Big]\, \Delta\varepsilon \end{aligned}$$

or, in the limit as $\Delta\varepsilon$ approaches 0

$$P\,(C = A) = \int_0^\infty P_Q\,(Q = \zeta) \cdot P_M\,(M = A/\zeta)\, d\xi$$

or

$$P_C\,(A) = \int_0^\infty P_Q(\zeta) \cdot P_M\,(A/\zeta)\, d\zeta$$

Expressing the operator above by *,

$$P_C = P_M * P_Q$$

This equation states that the probability density function for maximum ground-level concentrations can be derived from the convolution of the probability density functions for M and Q. Therefore, the frequency distribution of ground-level concentrations for an uncontrolled plant can be determined from determinations of M and Q.

Once P_C is known, the graphs corresponding to Figure 1 can be displayed, and the probability of violating standards is directly known.

Consider next the case when the SCS is operating. In this case $C_c = Q_c \cdot M$ where subscript c denotes the functional value when the SCS is operating. Q_c is no longer independent of meteorology since the operation of the SCS depends on meteorological forecasting.

P_Q will, therefore, also be generally dependent upon P_M and will vary for different control strategies. For computer solutions to the correlated integration, the dependence of these quantities upon each other can be readily simulated.

Assuming that the error ratio R is independent of M and of Q and given P_R, P_M, and P_Q it is possible to use the control strategy rules for determining Q_c to numerically evaluate P_{Cc} under the SCS control.

In this case $C_p = M \cdot Q \cdot R$. The value of Q_c is determined in each case from the predicted value of concentration C_p and from the strategy (e.g., strategy 1 or 2). From the resulting distribution of Q_c, the value of P_{Cc} is obtained from the equation

$$P_{Cc} = P_{Qc} * P_M$$

Note the parallel nature of this equation and the equation for P_C.

This means that the existing frequency distribution of ground level concentrations for a plant can be determined from archived measurements of Q and M, and from records of air quality forecasting accuracy during operational use of the SCS to determine R.

In practice, the determination of P_C is achieved by assuming that the values of Q and M are quantified so they can assume only a finite number of values. Therefore, P_Q and P_M represent probabilities rather than probability densities. The integral is then replaced by a numerical scheme which is solved on a digital computer. Similarly for the generation of P_{Cc}, the function R is assumed to be quantified and the probabilities of the quantified values of P_{Cc} are determined numerically. The numerical scheme employed by the ERT computer program to generate the above described frequency distributions can be modified to allow inter-dependence of Q and M. This property of the program is particularly valuable for operations where changes in effluent SO_2 emission rates may be associated with large changes in plume rise.

4. ANALYSIS OF RELIABILITY FOR SOME HYPOTHETICAL SCS SYSTEMS

4.1 Test Case Conditions and Assumptions

The ERT PROBL model has been applied to several hypothetical SCS operations to illustrate the utility of the probability analysis technique as well as to illustrate the dependence of the reliability of an SCS upon the various independent parameters which influence SCS reliability. Assumed input information is given as follows:

- The source is a singel 828-ft stack with the exit diameter, stack exit temperature, flue gas rate, and maximum SO_2 emission derived from data for a copper smelter operation.
- The meteorological input data was based on a 5-year stability-wind rose from the southwestern United States.
- Terrain is essentially ignored except for its effect on the stability-wind rose.

From the source data and the meteorological inputs detailed above, the Meteorology Function M and the Emissions Function Q can be defined. At any time, the Meteorology Function is predicted by the gaussian point-source diffusion model ERT PSDM for unit SO_2 emissions. The distribution of M is determined from the stability-wind rose. The maximum downwind PSDM model prediction for each weather condition is assigned the corresponding frequency from the stability-wind rose and the frequency distribution of M is constructed. The Emissions Function Q is assumed for these examples to be constant and equal to the full load emissions to simulate conditions in the absence of an SCS. The frequency distribution of Q is, therefore, very simple. The probability of full load is 1.0 and all other values have probability zero.

Specification of the SCS is accomplished through several parameters. A range of values for each parameter is considered in the examples below to represent all likely SCS operations.

Two SCS types are examined: (1) a single option switch plan, and (2) a continuous option switch plan. The single option plan is representative of fuel switching. Implementation of the SCS reduces emissions by the fraction β in all cases. The continuous option switch plan is representative of process curtailment. Implementation of the SCS reduces emissions by exactly that fraction necessary to reduce the maximum ground level con-concentration below a prescribed threshold. These two SCS types were chosen for study from an infinite set of SCS types which can be investigated by this probability analysis technique.

The distribution of the Error Ratio R is assumed to be a log-normal distribution well specified by a geometric mean value $\overline{R}$ and by the standard deviation of the distribution σ.

The characteristics of the distributions for R were chosen to be similar to the observed distribution of R described for the AIRMAP network in Figure 3. The log-normal shape and the width of each sample distribution are similar to those corresponding to this distribution. Error Ratio will be carefully specified for each example below.

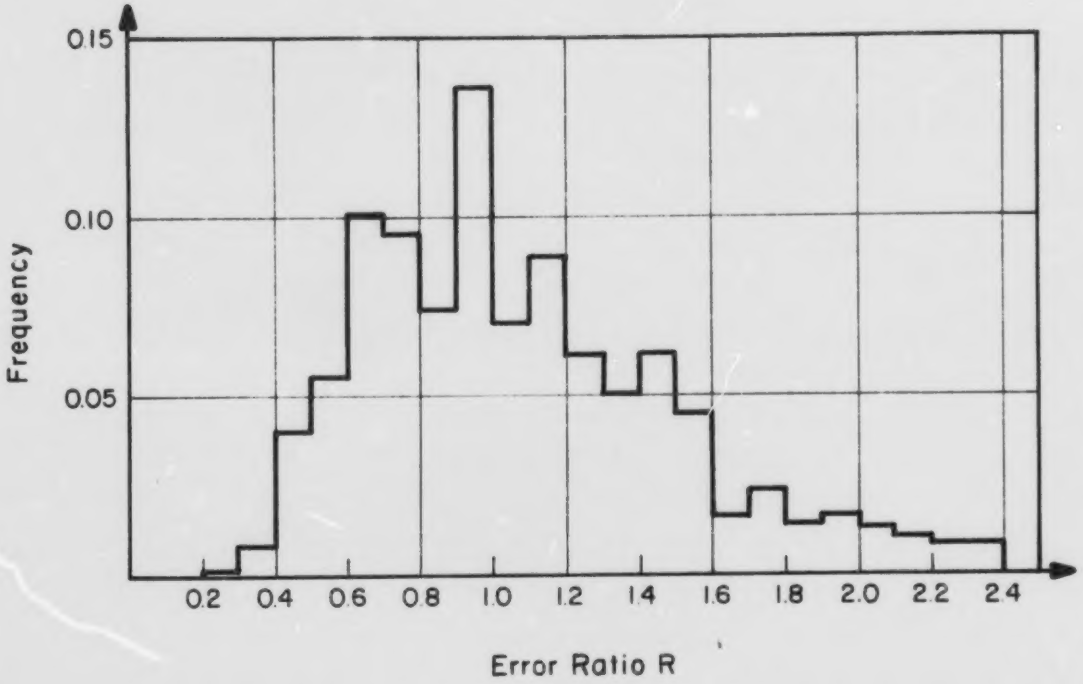
Each SCS, regardless of type, is assumed to have a switch threshold. If the predicted value of the maximum ground-level concentration is projected to exceed the switch threshold, the SCS emission reduction action is initiated. Obviously, the highest acceptable switch threshold is the air quality standard. Because of uncertainty in air quality forecasts, the switch threshold, γ, is usually some fraction of the standard.

4.2 Dependence of SCS Reliability on Various Influencing Factors

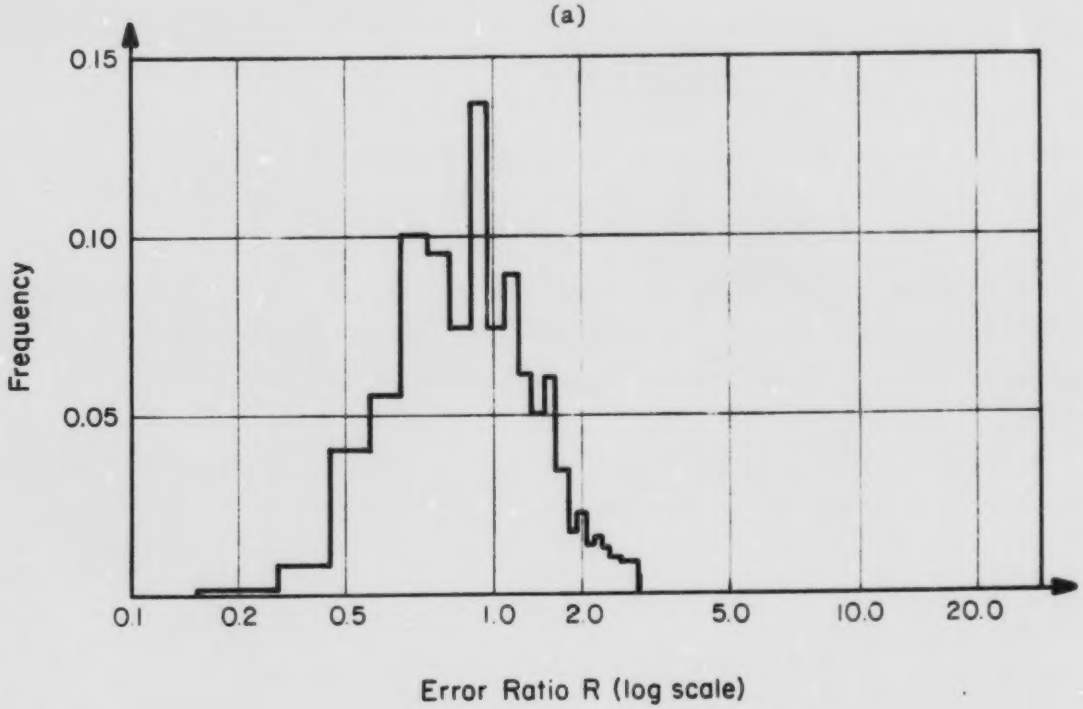
The following examples have been provided in order to isolate the effect of changes in each of the pertinent variables which influence reliability. These variables include: $\overline{R}$, the geometric mean of the error ratio R; σ, the standard deviation of the error ratio distribution; γ, the threshold value of the predicted maximum concentration above which some operational process adjustment is made; and β, the ratio of the sulfur content of the low sulfur fuel to the sulfur content of the high sulfur fuel used in a fuel switch SCS.

Example 1 - What is the effect on SCS reliability of changing the value of σ for the Error Ratio R?

Reduction of the value of σ for the Error Ratio R is a desirable objective of every SCS operation. If σ could be made negligibly small, the SCS could be perfectly reliable with a minimum loss of production or fuel costs for the source. A non-zero value of σ results from the presence



(a)



(b)

Figure 3 Distribution of the Error Ratio R for the Boston AIRMAP System

of unbiased errors in meteorological forecasting, estimation of emissions, or modeling results. A reduction in σ would be expected from any of the following system improvements:

- Additional or improved meteorological data used in predicting the meteorological parameters which are input for air quality forecasts. Unless R_w is very near 1.0 or the system is operating near the predictability limit for each parameter, some improvement through added meteorological support is expected. Among the possible improvements in meteorological support might be atmospheric sounding data, on-site wind measurements, NWS teletype or facsimile circuits, a wind field generator model, a faster data reduction system, or simply more frequent observations of important meteorological data.

- More experienced or more capable meteorological personnel. Because personnel gain experience as the system is operated, the σ of the system should become smaller with time.

- An improved model. As a forecasting model is updated through system experience, a reduction in σ is to be expected.

- An improved emission schedule forecast system. This improvement might be gained by more thorough production planning or it might involve more careful fuel or materials analysis, better emissions monitoring, or better plant process monitoring.

Table 4-1 summarizes the results of this example analysis. Note that all SCS operating parameters are the same for each SCS option except that σ is varied. The first column in the summary table describes the six SCS options and the NO SCS option (for comparison). The second column contains the frequency of violations of a 1-hour standard of 0.5 ppm expected to occur with the indicated control strategy. The third column contains the fraction of low cost fuel (higher sulfur content) which can be used. The remaining fraction of fuel must be more expensive (lower sulfur content) fuel. The fourth column contains the fraction of the time that full production is possible assuming that the SCS process curtailment is the only constraint.

Clearly, any of the six SCS plans reduces the frequency of violations by at least a factor of 2 but, interestingly, no more than a factor of 3.4.

Table 4-1

Effects on SCS Reliability of Changing the Value of σ for the Error Ratio R

Each SCS plan below has the following parameter values:

Fuel switching fraction $\beta = 0.25$

Switching threshold $\gamma = 0.5$

Geometric Mean of Error Ratio $\overline{R} = 1.0$

Width of Error Ratio distribution σ, is variable

SCS Control Strategy	Total Frequency of Violations	Fraction of Low Cost Fuel	Fraction of Time at Full Production
NO SCS	0.16432	1.000	1.000
SCS #1: FUEL SWITCHING σ = 0.5	0.06605	0.754	1.000
SCS #2: FUEL SWITCHING σ = 0.4	0.06291	0.768	1.000
SCS #3: FUEL SWITCHING σ = 0.2	0.04875	0.808	1.000
SCS #4: PROCESS CURTAILMENT σ = 0.5	0.08194	1.000	0.918
SCS #5: PROCESS CURTAILMENT σ = 0.4	0.08216	1.000	0.948
SCS #6: PROCESS CURTAILMENT σ = 0.2	0.08216	1.000	0.961

By improving forecast accuracy for the fuel switching cases, SCS reliability is noticeably improved. Since the fuel switching constant $\beta = 0.25$ is overly conservative in most cases, nearly every switch action results in concentrations below standards. Therefore, improved accuracy of prediction (reduced σ) results in fewer potential violations escaping control. Since the switch threshold $\gamma = 0.5$ is exactly the standard, there is no conservatism in the process curtailment forecasts. Although improved forecast accuracy reduces the magnitude of violating concentrations, the number of violations remains the same. These examples indicate that some conservatism is desirable for an efficient SCS strategy. Ways of including conservatism are discussed later.

Improved forecast accuracy can have possible economic and social benefits despite the probable added expense. For the fuel switching examples, use of valuable low sulfur fuel is reduced from .25 to .23 and finally to .19 of the total fuel used as forecasting accuracy is improved. Meanwhile, SCS reliability is also improved. Note that full production is assumed to be possible regardless of fuel type. For the process curtailment cases, the percentage of full production is increased as forecast accuracy improves. Meanwhile, SCS reliability is maintained at the same level.

Example 2 - What is the Effect on SCS reliability of changing the value of $\overline{R}$ for the Error Ratio R?

The geometric value of the Error Ratio, $\overline{R}$, is less than 1.0 if concentrations are characteristically underpredicted, greater than 1.0 if concentrations are characteristically overpredicted, and 1.0 if there is no systematic bias in prediction. It is easy for a system to achieve a value of $\overline{R} = 1.0$ by simply reducing each forecast value by the required amount to bring the mean of past values to 1.0. It is generally desirable, however, to intentionally operate an SCS conservatively to prevent a high frequency of violations which are near but higher than the standard. The limits on reliability of a nonconservative SCS were illustrated in the previous example analysis. One method of operating a conservative SCS is to maintain an Error Ratio mean $\overline{R}$ greater than 1.0.

An air quality forecast model which overpredicts provides a means of achieving $\overline{R}$ greater than 1.0. Most air quality models overpredict because "worst case" conditions such as persistent meteorology and conservative plume rise are assumed.

Similarly, meteorological and emission predictions used for air quality projections are often chosen to be "worst case" forecasts. For example, predicting fumigation conditions for all clear mornings would produce a value of $\overline{R}$ greater than 1.0, but may be necessary to prevent contravention of standards on those several mornings when inversion breakup is a problem.

The example analysis which follows is designed to investigate the effect of changing $\overline{R}$ on SCS reliability, leaving all other SCS parameters unchanged. Table 4-2 includes the results of the operation of six hypothetical SCS schemes and the NO SCS case.

Again, each of the six SCS plans reduces the frequency of violations by a considerable amount. The increased conservatism of air quality prediction, manifested in increased values of $\overline{R}$, reduces the frequency of violations of the standard for both fuel switching and process curtailment. For fuel switching, 43 of every 44 violations can be eliminated using an SCS with $\overline{R} = 2.0$.

The economic penalty for the indicated improvements in air quality is shown in the final two columns of Table 4-2. With $\overline{R} = 2.0$, lower sulfur fuel is required 59% of the time for operation of the fuel switching plan. For process curtailment, a negligible violation frequency is accomplished by reducing maximum possible production by 39%. Unlike reducing σ, increasing $\overline{R}$ above 1.0 has no compensating economic savings.

The preceeding examples are illustrative of the types of analyses which can be prepared to investigate the impact of various SCS parameters on system reliability and on low sulfur fuel usage. A more extensive presentation of the sensitivity of these factors on system parameters may be found in Reference 1.

4.3 Quantitative Separation of SCS Component Errors

ERT has developed a working procedure for evaluating the uncertainty of meteorological forecasting and of air quality modeling during the operation of an SCS. The procedure requires that the following three concentration values be recorded for each forecasting time:

- The model predicted concentration using predicted meteorological and emission parameters. (This concentration value is the basis of the SCS control action which will affect concentrations T hours later.)

Table 4-2

Effects on SCS Reliability of Changing the Value of $\overline{R}$ for the Error Ratio R

Each SCS plan below has the following parameter values:

Fuel switching fraction = $\beta = 0.25$
Switching threshold = $\gamma = 0.5$
Geometric mean of error ratio $\overline{R}$ is variable
Width of error ratio distribution $\sigma = 0.5$

SCS Control Strategy	Total Frequency of Violations	Fraction of Low Cost Fuel	Fraction of Full Production
NO SCS	0.16432	1.000	1.000
SCS #1: FUEL SWITCHING $\overline{R} = 1.0$	0.06606	0.754	1.000
SCS #7 FUEL SWITCHING $\overline{R} = 1.5$	0.00876	0.521	1.000
SCS #8: FUEL SWITCHING $\overline{R} = 2.0$	0.00370	0.413	1.000
SCS #2: PROCESS CURTAILMENT $\overline{R} = 1.0$	0.08194	1.000	0.918
SCS #9: PROCESS CURTAILMENT $\overline{R} = 1.5$	0.01306	1.000	0.836
SCS #10: PROCESS CURTAILMENT $\overline{R} = 2.0$	0.00000	1.000	0.609

8260

- The model predicted concentration using observed meteorological parameters and predicted emissions.
- The model predicted concentration using observed meteorological and emission inputs.
- The maximum concentration recorded by the monitoring network.

The procedure combines the above recorded data in a way which isolates the error in air quality forecasting due to meteorological forecasting uncertainty from the error due to model uncertainty.

Recall the formulation developed in Section 3 for ground level concentration:

The observed maximum concentration is assumed to be $C_o = Q_o \cdot M_o$

The predicted maximum concentration is assumed to be $C_p = Q_p \cdot M_p$

where the Error Ratio R is the ratio

$$R = C_p/C_o$$

R is a function which contains contributions from all sources of error and uncertainty which prevent a perfect air quality forecast; that is, $C_p = C_o$. These sources of uncertainty arise from each component of the SCS -- meteorological forecasting, emissions forecasting, and air quality modeling. Consider the following formulation of R:

$$R = R_w \cdot R_q \cdot R_m$$

where R_w, R_q, and R_m are the error ratios for meteorological (weather) forecasting, emissions prediction, and air quality modeling respectively.

It is clear that,

$$\frac{C_p\ (Q_p,M_p)}{C_p\ (Q_p,M_o)} \cdot \frac{C_p\ (Q_p,M_o)}{C_p\ (Q_o,M_o)} \cdot \frac{C_p(Q_o,M_o)}{C_o} = R$$

Where $C_p\ (Q_p,M_p)$ is there predicted concentration using predicted meteorological parameters and predicted source emissions, $C_p(Q_p,M_o)$ is the predicted concentration using predicted source emissions and observed meteorological parameters and $C_p(Q_o,M_o)$ is the predicted concentration using observed source emissions and observed meteorological parameters.

That is, the error ratio R can be expressed as the product of three ratios representing the weather forecasting, emissions, and air quality model ratios of predictions-to-observations.

In order to meet the EPA requirements for documentation of the SCS reliability, it is necessary to undertake a detailed test program to continuously collect air quality data for purposes of establishing system reliability.

To assess system reliability, it will be necessary to measure the reliability of the individual components of the SCS decision making process. Records of the predicted meteorological parameters, predicted emission rates and predicted SO_2 concentration levels will be continuously recorded. These data in conjunction with observed meteorological data, emissions data, and measured concentrations provide sufficient information to separate meteorological forecasting uncertainty, emissions forecasting uncertainty and air quality modeling errors. The analysis scheme described in this section is designed for this application. After the test period of real-time operation of the SCS, a study of the magnitude of these individual uncertainties and a study of the consistency of these errors will be a valuable measure of system reliability.

Since federal regulations consider reliability to be defined as the probability that an SCS will not violate air quality standards, it is informative to generate the frequency distribution for maximum ground-level concentrations. Using the analysis scheme developed in Section 3, the frequency distributions of Q, M and R can be generated during the test period to define the probability that air quality standards will not be violated.

In summary, then, the test program can consist of continuous real-time operation of the system, recording of all predicted parameter values, recording of all measured parameter values, and the determination of system reliability based on the analysis programs of Section 3. These results in conjunction with a detailed description of all elements of the SCS can be submitted to the control agency as demonstration of the ability of the system to meet standards.

EPA regulations authorize control agencies to deny continued use of the SCS if the source fails to refine and upgrade the response of the SCS to adverse dispersion conditions. The isolation of modeling errors by the techniques described in this section can be used to update the air quality prediction model. Systematic modeling errors can be used to develop calibration factors for the models which should improve system reliability as system experience accumulates. Also, isolation of the meteorological uncertainty is a valuable indicator of improvements which might be made in the forecast system. Finally, the probability of violating standards can be generated periodically as the emission, background, and accuracy of the system changes with time. This periodic check on system performance assures that system reliability can be maintained and, ideally, improved as operators gain experience with the system.

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Chapter 29

ON THE LOGNORMAL DISTRIBUTION OF AIR POLLUTION DATA

by

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on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

29-2

On the Lognormal Distribution of Air Pollution Data

by

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Air pollution concentrations, because of their natural cutoff at zero, usually have a skewed frequency distribution. Larsen (1,2) has proposed that air pollutant concentrations are lognormally distributed for all averaging times. Kahn (3) has proposed a justification for Larsen's use of the lognormal distribution by deriving it as one of a class of distributions first proposed by Kapetyn (4). The derivation goes as follows; if air pollution concentrations are thought to be a function of many random processes occurring simultaneously, changes in air pollution concentrations may be represented by equation (1)

$$X_{i+1} - X_i = Pi\ g(Xi) \qquad (1)$$

where Pi is a random variable representing the stochastic nature of the processes and g(Xi) is some unknown function of the concentration Xi. For small concentration changes,

$$X_{i+1} - Xi = dXi \qquad (2)$$

Integrating equation 1 leads to

$$\int_{Xo}^{Xn} \frac{dXi}{g(Xi)} = \sum_{i=0}^{n-1} Pi \qquad (3)$$

If g(Xi) is assumed to be a constant X_d plus the concentration Xi one arrives at the relation

$$\ln(X_d + Xn) = \ln(X_d + Xo) + \sum_{i=0}^{n-1} Pi \qquad (4)$$

For a sufficiently large n the correlation coefficient between Xn and Xo becomes zero, and for many samples of averaging time n, by the Central Limit Theorem, the log of (X_d+Xn) becomes normally distributed.

The lognormal distribution of concentration is therefore a special case for $X_d = 0$, since the distribution becomes normal as X_d becomes large. The lognormal hypothesis was tested by analysis of air pollution data to determine whether the value of X_d which best fit the data was indeed zero. In almost all cases examined covering different pollutants form different countries it is evident that experimental data are indeed better fit using finite positive values for X_d, greater than the arithmatic mean of the distribution.

Figure 1 shows data for SO_2 from Washington D.C. reported by Larsen (1). These 12-hour average values fall on a straight line on logprobability paper when the concentration is transformed by the addition of 0.10 ppm to each measured concentration. Figure 2 shows data on NO_2 from France (5), also linearized. Figure 3 shows data from Germany (6) for CO, again linearized by the same transformation. In each case the added constant is greater than the arithmatic mean $\bar{X}$. Analysis of the data also indicates that the constant X_d depends upon the averaging time. Figure 4 shows data for SO_2 from Washington D.C. from the same source cited for Figure 1, but for a one-hour averaging time. In this figure the constant added is 0.05 ppm as compared with 0.10 ppm for the 12-hour average data. The arithmatic mean $\bar{X}$ of the distribution computed by the formula shown as equation 5 is approximately .045 ppm SO_2.

$$\bar{X} \cong \sum_{0}^{1.00} X(\Delta f) \qquad (5)$$

Extrapolation back to averaging time equal zero indicates that for this limiting case the constant to be added is the mean itself. Preliminary indications thus show that the term X_d can be represented as a constant k times the mean $\bar{X}$, ($X_d = k\bar{X}$), where k is a dimensionless variable that increases with averaging time from a value of unity. The author is presently developing the theoretical model to explain this transformation and behavior of the variable k.

The transformation described in this paper is classified by Aitchison and Brown (7) as a three parameter lognormal distribution censored at the third parameter. The distributions end at $X = k\bar{X}$ in a vertical line to prevent the extension into the negative concentration domain. The transformation also provides the physical significance to prevent the maximum concentration, as frequency goes to 100%, from becoming greater than that permitted by the 2nd Law of Thermodynamics (10^6 ppm).

The transformation described may not be applied to the data when they indicate a violation of the 2nd Law in the untransformed state. An example of such a case is shown in Figure 5, in which the results of 26 random samples for Chromium were taken during a year (8). The downward curvature of the data indicates a violation of the 2nd Law and the author has extended the line upward to show the curvature required by theory. This type of distribution is caused by the sampling of a nonuniform distribution of sources. When an overriding large source is very close to the monitoring station two separate and identifiable distributions may be shown to exist. One when the wind blows from the monitoring station to the source (I) and the second when the wind is from the source to the monitoringstation (II). The distribution may be decomposed into two different distributions by statistical techniques described by Hald (9). After obtaining the two distributions, a different value of k may be used for each, and the two component distributions may be plotted as shown on Figure 5.

In conclusion, air pollution data may be treated by assuming that the function ($X + k\bar{X}$) is lognormally distributed, with the dimensionless parameter k determined by goodness of fit.

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FIG. 1

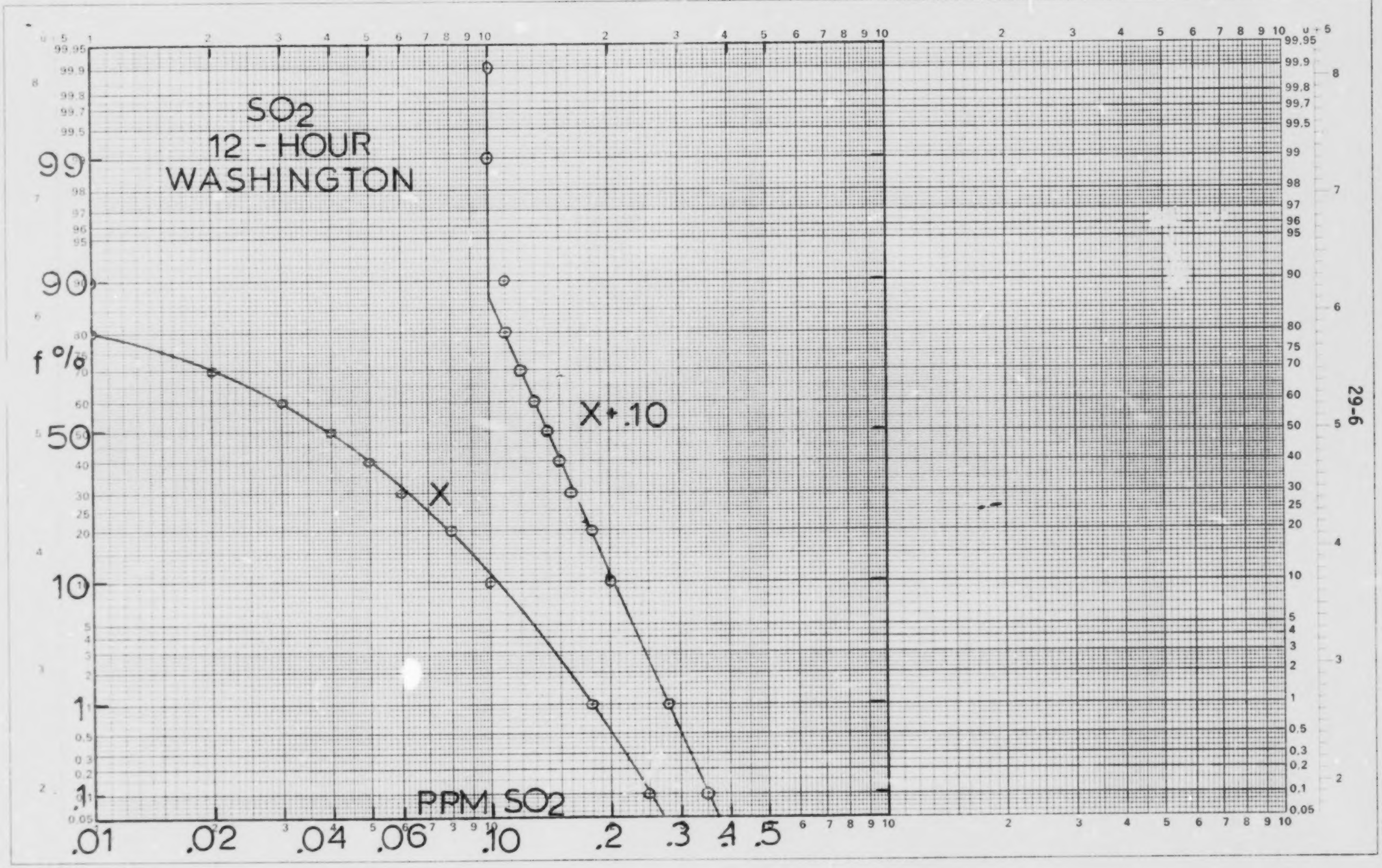
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FIG. 2

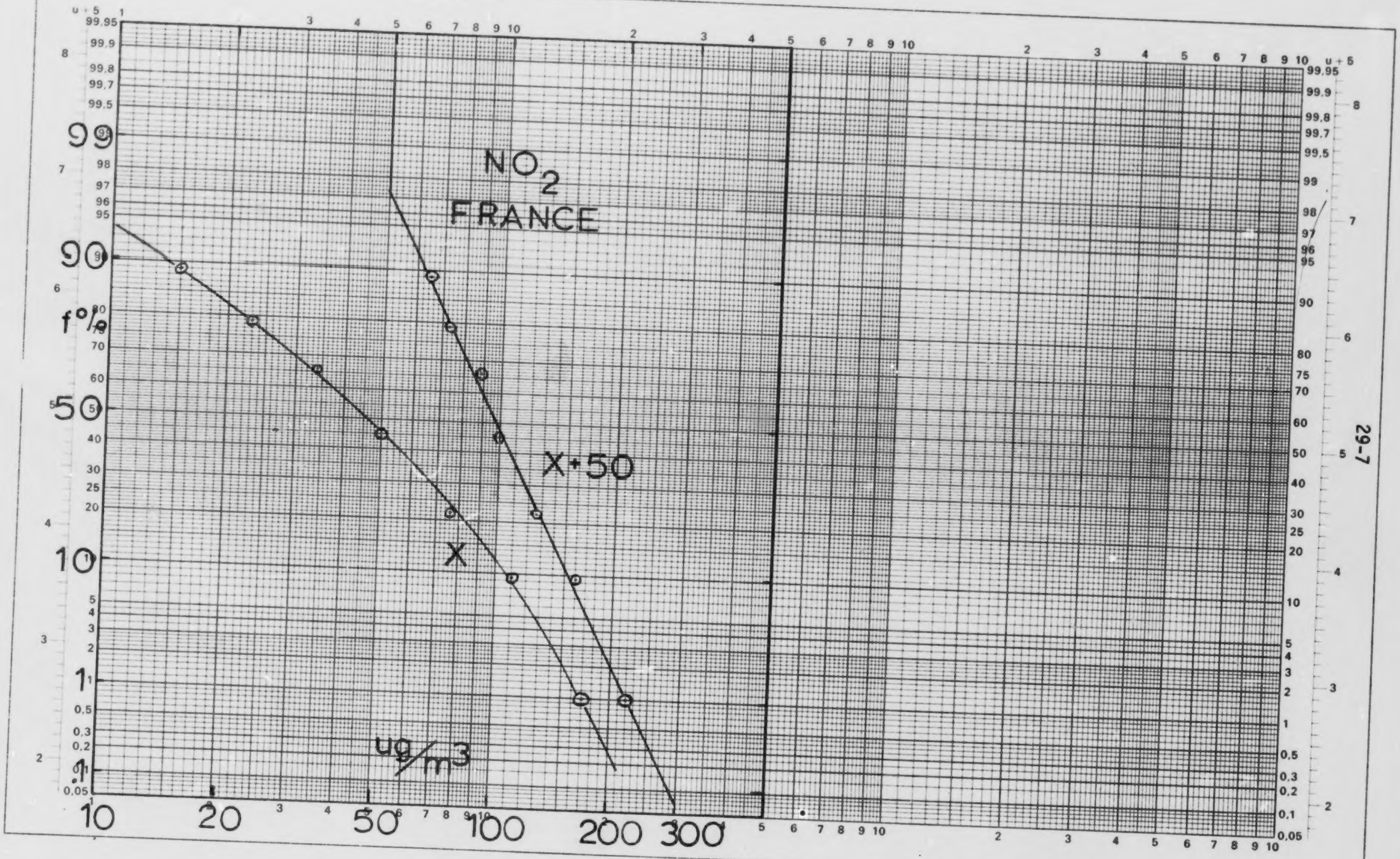


FIG. 3

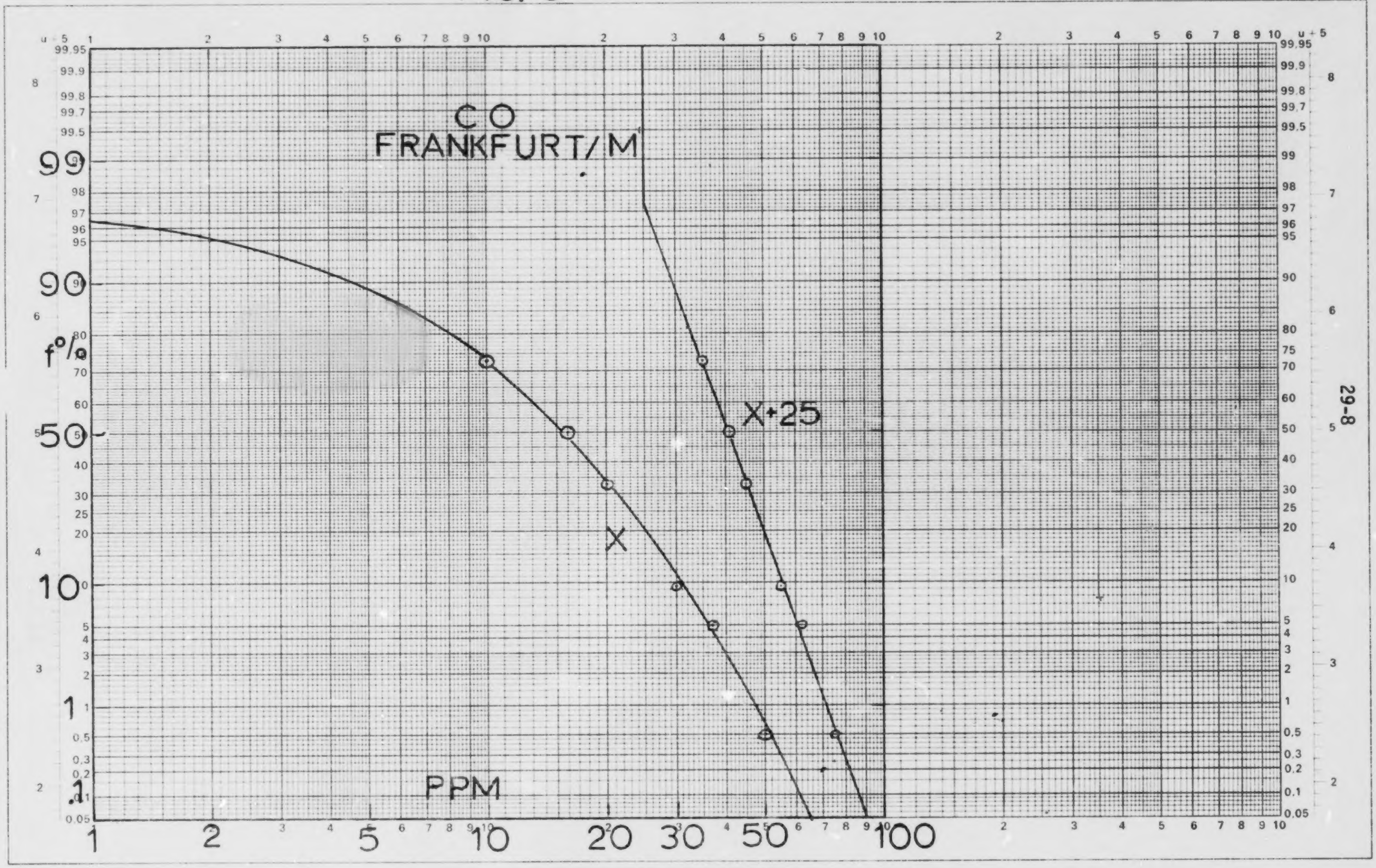
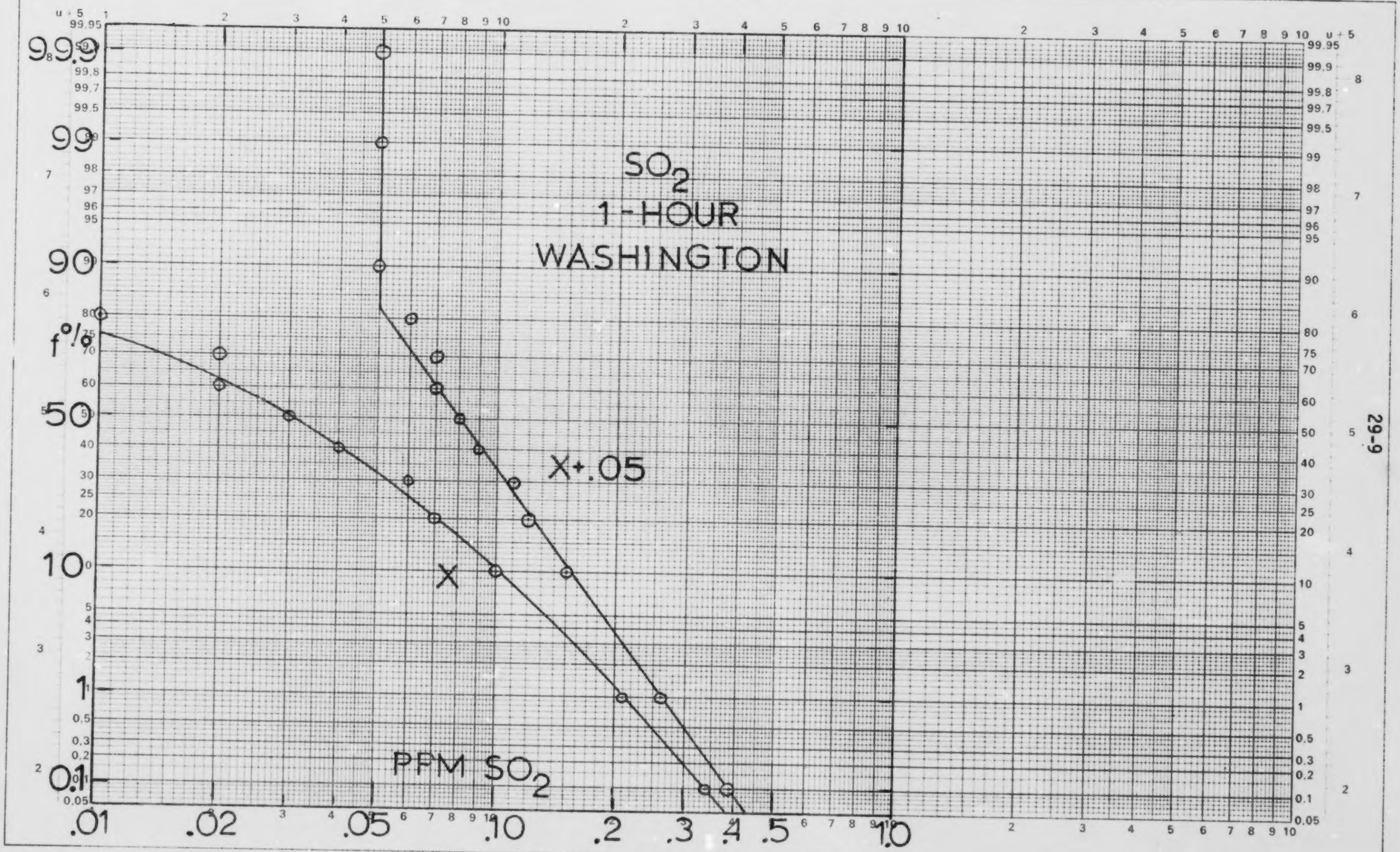


FIG. 4



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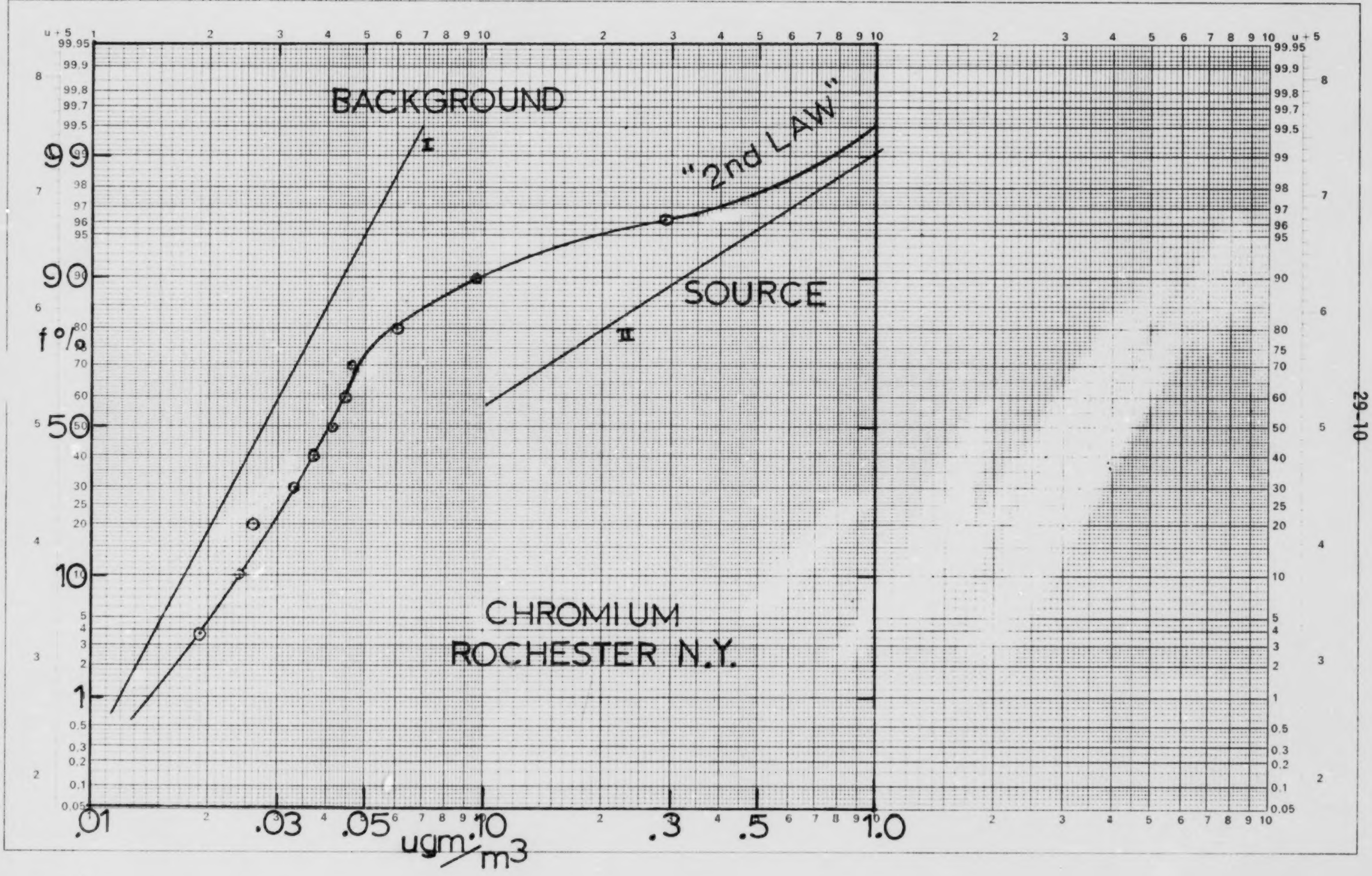
1.0
29-9

FIG. 5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SOURCE
II
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ROCHESTER N.Y.
f%
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10
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.01
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.05
.10
.3
.5
1.0
ugm/m3

Chapter 30

STATISTICAL DESCRIPTION OF AIR POLLUTION CONCENTRATION, AVERAGING TIME AND FREQUENCY

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

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Roskilde, Denmark
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STATISTICAL DESCRIPTION OF AIR POLLUTION CONCENTRATION, AVERAGING TIME AND FREQUENCY

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Summary

The paper discusses an empirical model for the relation between air pollution concentration frequencies and averaging time, which has been proposed by R.I. Larsen and others. The model can be formulated in terms of two "laws", Larsen (1969).

1. Concentrations are approximately lognormally distributed for all pollutants in all cities for all averaging times.
2. The median concentration is proportional to averaging time to an exponent (and thus plots as a straight line on logarithmic paper).

The model is illustrated on fig. 1, which is taken from Larsen (1969). A closer inspection of fig. 1, and other plots like this, shows that although the model approximates the behaviour of the data fairly well, it is just as evident that there are systematic differences between the model and the data too.

With the data from fig. 1 as test data we have studied the behaviour of the concentration statistics with averaging time, by bringing it into relation with time series statistics for the pollutant time series. We have used Larsen's "first law" about lognormality, while to describe the variation with averaging time we have used the behaviour of the sample variance with averaging time for a stationary stochastic time

series, i.e.

$$s_T^2 = \frac{2s^2}{T} \int_0^T (1-\frac{t}{T})\ \rho(t)dt = \int_{-\infty}^{\infty} (\frac{\sin\ \omega T/2}{\omega T/2})^2\ S(\omega)d\omega, \quad (1)$$

where s_T^2 is the sample variance of the averaged series with averaging time T, s^2 is the variance of raw data, $\rho(t)$ is the autocorrelation function, and $S(\omega)$ is the power spectrum of the pollutant time series.

With a known $\rho(t)$, knowledge about s_T^2 and the mean value of the series, $\bar{x}$, for a given averaging time enables one to determine the sample variance for all averaging times. Thereafter the two parameters in the lognormal distribution, σ_T and μ_T, can be determined through

$$\begin{aligned} \sigma_T{}^2 &= \ln(s_T^2/\bar{x}^2+1) \\ \mu_T &= \ln(\bar{x}/\sqrt{s_T^2/\bar{x}^2+1}), \end{aligned} \quad (2)$$

and the concentration level x_{pT} corresponding to any percentile of the order p can be determined through

$$x_{pT} = e^{\mu_T + y_p\sigma_T} \quad (3)$$

where y_p is the corresponding percentile for a standard normal distribution.

The expected maximum and minimum values are estimated by estimating the corresponding p's by

$$p_{max} = \frac{1}{n+1} \text{ and } \quad p_{min} = \frac{n}{n+1}, \quad (4)$$

where n is the number of independent observations in the data series.

For simplicity we have used an exponential autocorrelation function, with the time constant τ.

$$\rho(t) = e^{-|t|/\tau}. \qquad (5)$$

When using eqs. 1 through 5 the behaviour of the percentiles with averaging time is shown in fig. 2.

In fig. 3 the data shown in fig. 1 are shown again, but with an expanded ordinate. The curves in fig. 3 are generated with an exponential autocorrelation function with a six-hour time constant.

The only deviation from the scheme described above is due to the fact that the instrument used to obtain the data has a time constant λ=10 min., Larsen (1969). For this reason (1) has been used in the form:

$$s_T^2 = \frac{2s^2}{T+\lambda} \int_0^{T+\lambda} (1-\frac{t}{T+\lambda}) \, e^{-|t|/\tau} dt. \qquad (6)$$

n in (4) has been determined through

$$n = K_T \frac{T_o}{T+2\lambda} \qquad (7)$$

where K_T takes into account that not all data are available for a given averaging time, Larsen (1969). T_o is the length of the total series.

Fig. 3 shows that the curves fit the data well for averaging times less than a day, while they for longer averaging times underestimate the deviation from the mean. In fig. 4 the maximum values and the 10% percentiles are isolated to illustrate this point. The solid curves are the same as in fig. 3. The broken curves are calculated using a correlation function with a larger tail:

$$\rho(t) = 0.85\, e^{-|t|/\tau_1} + 0.15\, e^{-|t|/\tau_2} \qquad (8)$$

where τ_1 = 6 hours and τ_2 = 360 hours.

The small circles on the figure display the variation of the maximum values if the instrumental response time is neglected.

Fig. 5 shows that (8) may actually be a good approximation for many pollution data. The autocorrelation function shown on this figure may approximately be decomposed into a sum of two exponential functions with the same time constants as in (8). Fig. 6 shows the logarithmic power spectrum of airpollution data from Copenhagen. This spectrum shows a strong seven-day-periodicity in the data. The effect of such a periodicity on the diagram of percentiles and extreme values versus averaging time is shown in fig. 8, where it is seen that the data make a jump at seven days. This can be explained for instance in terms of the spectral form of (1), where it is seen that the spectral window, $(\sin(\omega T/2)/(\omega T/2))^2$, suddenly will cut away the contribution to s_T^2 from this peak, when T increases to above seven days.

Conclusion

The purpose of the study above has been to draw attention to the possibilities of statistical time series analysis on the pollution data, especially in this context to the possibility of using spectral (or correlation function) analysis as means to validate and probably refine R.I. Larsen's model.

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Prinz, B., Untersuchung zeitlicher Immisionverläufe mit Hilfe spectralanalytischer Metoden, Staub-Reinhalt, Luft 32, 26-29 (1972).

(The complete paper is in the proceeding from the AMS/WMO Symposium on Atmospheric Diffusion and Air Pollution, Santa Barbara, Sept. 9-13, 1974).

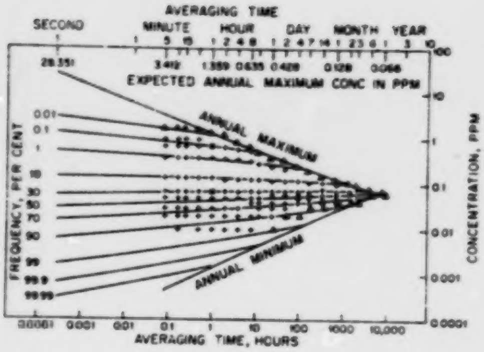

Fig. 1. Concentration vs. averaging time and frequency for Nitrogen Oxides in Washington D.C., Larsen (1969).

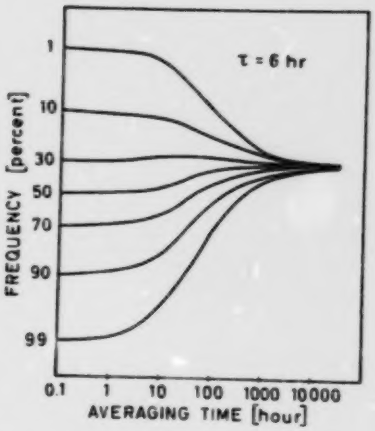

Fig. 2. Percentiles vs. averaging time, assuming an exponential correlation function with a six-hour time constant.

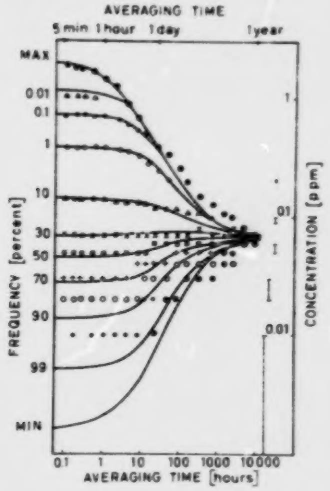

Fig. 3. Concentration vs. averaging time and frequency, same data as in fig. 1. The curves are based on an exponential correlation function with a six-hour time constant. The vertical beams describe the resolution of the data.

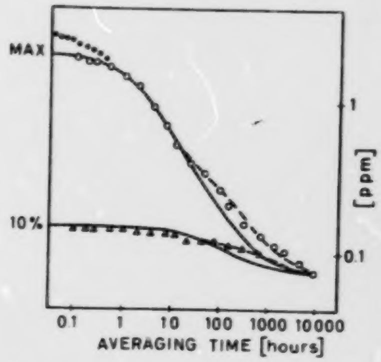

Fig. 4. Maximum values and 10% percentiles from fig. 3, O: Measured max.values, Δ : Measured 10% percentiles, o: Calculated curve neglecting the instrumental response time, ——: Calculated curve assuming the correlation function to be a single exponential function, -----: assuming it to be the sum of two exponentials.

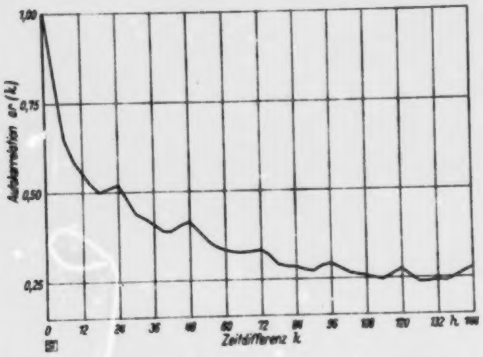

Fig. 5. Autocorrelation for SO_2 measurements in Düsseldorf, Prinz (1972).

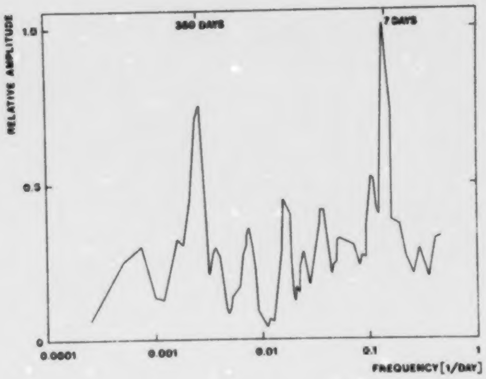

Fig. 6. Logarithmic power spectrum of measurements of air-borne particulate material from Copenhagen, Lyck and Gryning (1972).

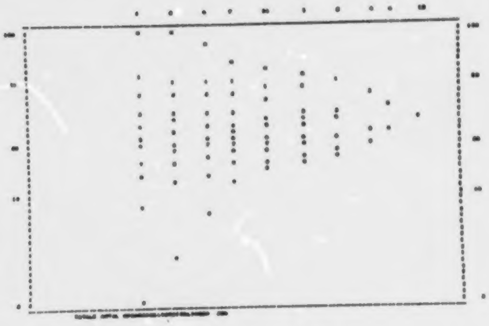

Fig. 7. Concentration vs. averaging time and frequency for the same data as in fig. 6.

Chapter 31

FLUID MODELING PROGRAM OF THE METEOROLOGY LABORATORY, U. S. ENVIRONMENTAL PROTECTION AGENCY

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

INTRODUCTION

This paper briefly reviews the recent efforts of the Meteorology Laboratory (ML), Environmental Protection Agency, in dealing with complex flow situations.

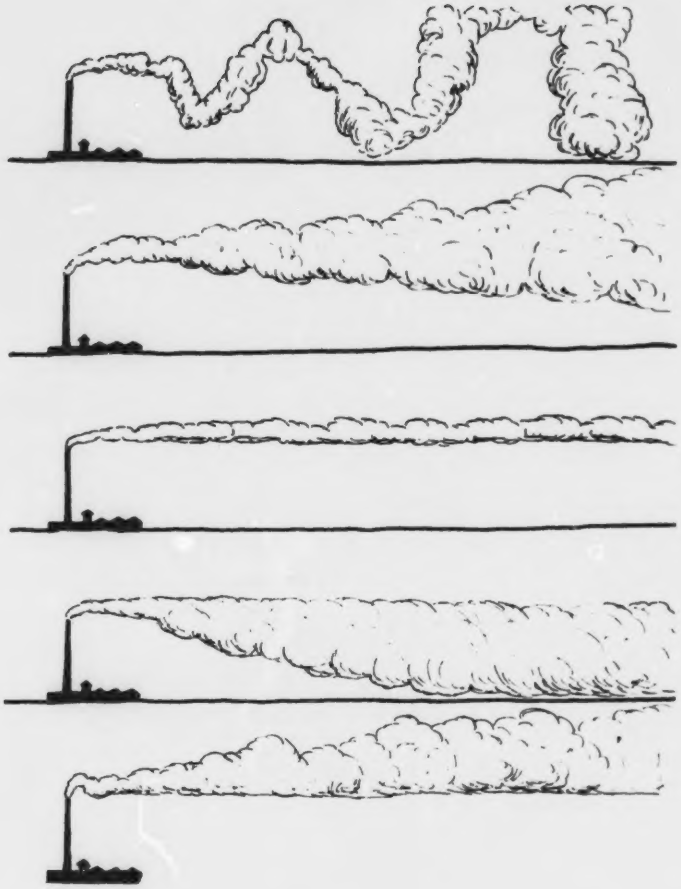
Section I consists of a recent brochure prepared for visitors to the newly acquired Meteorological Wind Tunnel. It describes the salient features of the new facility and gives examples of anticipated applications.

Section II describes some stack downwash studies conducted in a smaller wind tunnel. Section III covers a wind tunnel study of negatively buoyant plumes done on a grant from EPA. Section IV shows some results of a numerical model of flow and diffusion in a street canyon done on contract to EPA. Section V gives some preliminary results of a cooperative water channel/field study of plume diffusion in complex terrain done by the French Meteorological Service, Securipol, and EPA. Finally, Section VI gives the highlights of a towing tank study of plume diffusion under stably stratified flow conditions in complex terrain done on contract to EPA.

I. THE EPA METEOROLOGICAL WIND TUNNEL PROGRAM

Introduction

Through the Clean Air Act as amended in 1970, the Environmental Protection Agency is charged with the responsibility of determining the concentration of pollutants in the atmospheric boundary layer. A primary responsibility of the Meteorology Laboratory is the development and evaluation of atmospheric diffusion models for this purpose. Previously, the Laboratory's Model Development Branch has carried on these efforts with field studies and mathematical programs. Because of the limitations of these methods, a new Fluid Modeling Program has been established. It includes a Meteorological Wind Tunnel with associated facilities and a complete staff to aid in the solution of complex flow situations. This brochure describes the salient features of the new facility and gives examples of some typical applications.



DIFFUSION IN THE ATMOSPHERE

Wind in the atmosphere is a highly complex phenomenon: the only absolute certainty about the wind is that it is always changing. In the earth's boundary layer, the average wind speed increases from zero at the ground to its maximum value at an altitude of typically 700 m. Both its speed and direction change with time, from one instant to the next, from one hour to the next, and from one day to the next. Meteorologists have found that wind effects can be separated roughly into two scales of motion: large scale motions whose time periods are greater than a few hours, and small scale motions with time periods smaller than an hour. The large scale motions are called weather; the small scale ones, are called turbulence. Often one can visualize this separation of scales by studying a plume from a smoke stack for a period of time. At any given instant, the centerline of the plume will form a reasonably straight line (after its initial bending over and in the absence of obstructions to its motion). This straight centerline is indicative of a reasonably constant wind direction for at least the duration of time it took the farthest visible portion of the plume to get to its position after it left the stack. However, the plume spreads as it travels downwind. This spreading is caused by the smaller scales of motion, which are called gusts, eddies, or more generally, turbulence. It is these smaller scales of motion, with the mean wind speed and direction over a one hour or so time period remaining constant and where the turbulence contributes to the spreading of a plume, that can be simulated in a meteorological wind tunnel. The rate of dilution in the plume, however, can vary drastically from one day to the next, given identical wind speed and direction. The variability is related to atmospheric stability coupled with solar heating of the ground, and results in plume looping, coning, fanning, or lofting characteristics. Specifying the stability as well as wind speed and direction, the plume behavior may still be drastically different if a tall building or hill were placed in the vicinity of the stack.

METHODS FOR PREDICTING POLLUTANT FLOW AROUND STRUCTURES*

	MATHEMATICAL MODELS	FLUID MODELS	FIELD PROGRAMS
ACCURACY	GOOD	BETTER	BEST
RESOLUTION	COARSE (20M)	INTERMEDIATE (3M)	FINE (1M)
TIME	SMALL (2-4 WEEKS)	SMALL (2-4 WEEKS)	LARGE (1 YR)
COST	MODERATE ($25K)	SMALL ($10K)	LARGE ($100K)

*THE NUMBERS REPRESENT ONLY ROUGH ESTIMATES (COMPARATIVE ORDERS OF MAGNITUDE) FOR A VERY SPECIAL SET OF CIRCUMSTANCES. THEY MAY NOT BE USED FOR INTERPOLATION, EXTRAPOLATION, OR IN ANY OTHER WAY AS A BASIS FOR ESTIMATION.

WHY MODEL IN A WIND TUNNEL?

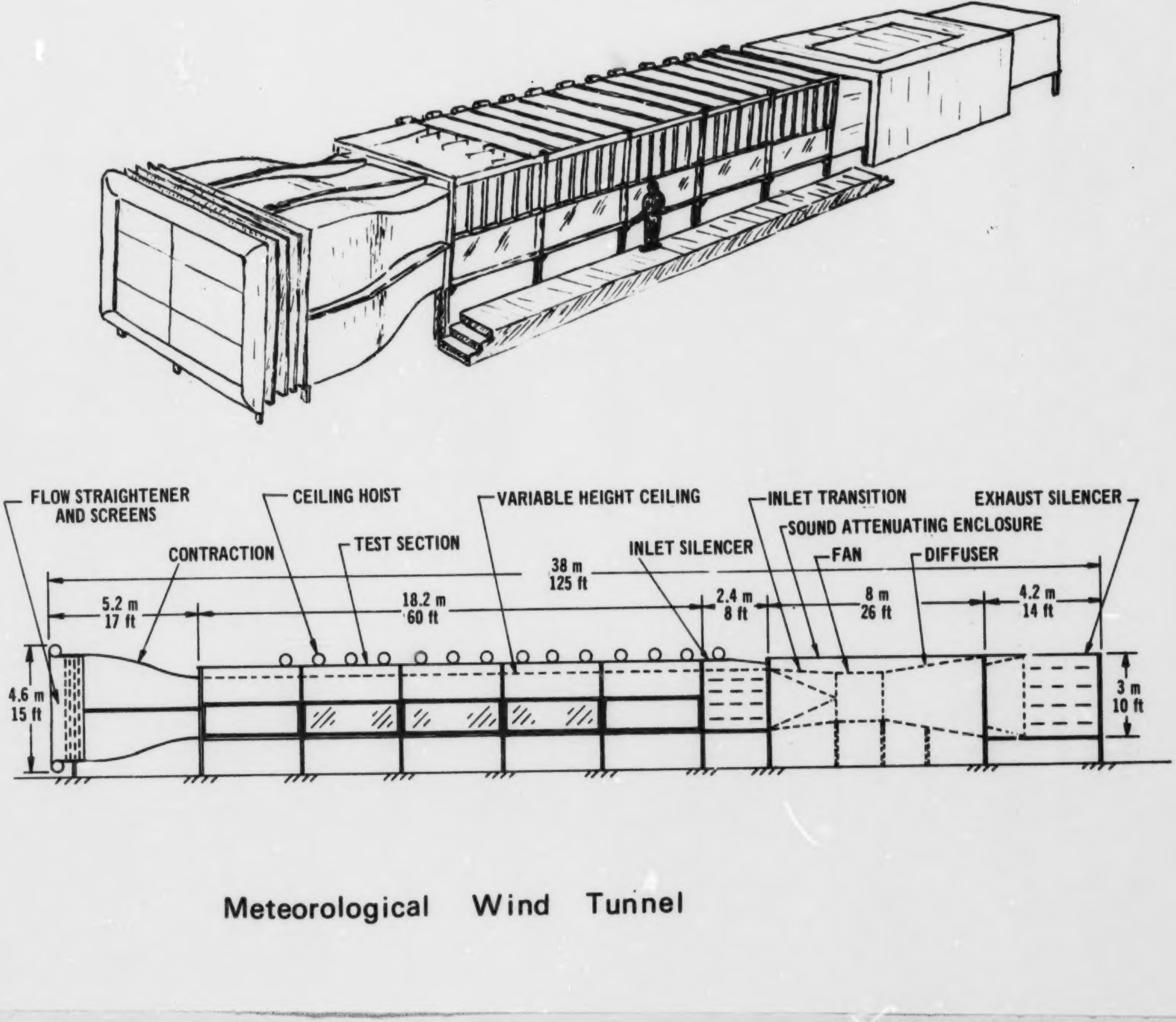
Given stack effluent characteristics, how does one go about predicting the likelihood of exceeding the Air Quality Standards at ground level? There are basically three methods which can be used: field programs, mathematical models, and fluid models.

Numerical models lend themselves to evaluation of alternate strategies but they require gross simplifications. The fundamental fluid dynamical processes involved in the dispersion of materials are not sufficiently understood and computer memories are still far too small to keep track of the detailed eddy motions in the atmospheric boundary layer so that these models are not exact. Present mathematical models are not yet adequate for calculating concentrations of contaminants when the plume is strongly affected by obstructions.

Field programs apparently provide the most believable results. However, they are very expensive, time consuming and fickle. Meteorological conditions are not controllable and often do not cooperate; a long time (greater than 1 year) must be spent in the field to obtain a proper range of conditions and even then specific sets of conditions may not occur. It is impossible to investigate the impact of potential source changes in alternate implementation strategies using field programs.

Fortunately, fluid models appear to work best where mathematical models fail, that is, where obstructions such as buildings and hills block the flow. Fluid models show great promise for simulating surface induced flows such as heat island circulation and mountain-valley winds. A fluid model has programmed atmospheric conditions so that years of field time are reduced to weeks.

Fluid model studies can reduce the resources required for field studies as well as aid significantly in their design. They are able to improve the development of better mathematical models by filling in gaps in the present models. A complete program includes comparisons and feedbacks between all three methods -- fluid models, mathematical models, and field programs -- in order to gain deeper understanding of the complex processes associated with atmospheric transport and diffusion of contaminants.


FLOW STRAIGHTENER AND SCREENS
CEILING HOIST
VARIABLE HEIGHT CEILING
INLET TRANSITION
EXHAUST SILENCER
SOUND ATTENUATING ENCLOSURE
CONTRACTION
TEST SECTION
INLET SILENCER
FAN
DIFFUSER
38 m 125 ft
5.2 m 17 ft
18.2 m 60 ft
2.4 m 8 ft
8 m 26 ft
4.2 m 14 ft
4.6 m 15 ft
3 m 10 ft

Meteorological Wind Tunnel

HOW CAN THE FLUID MODELING PROGRAM HELP SOLVE YOUR PROBLEMS?

The Meteorological Wind Tunnel, one of only a few atmospheric dispersion modeling facilities in the world, is available to other branches of EPA, to EPA Regional Offices, to state air pollution control agencies, and to other branches of the federal government. The fluid modeling program is designed to provide fast response to questions arising in the area of pollutant dispersal in complex flow situations. Our fluid modeling program consists of the Meteorological Wind Tunnel, model shop, electronics shop, darkroom, chemical laboratory, and mini-computer, including disc, magnetic tape drives, electrostatic printer/plotter and CRT display. Various electronic, mechanical and chemical equipment is available for metering and measuring flows and concentrations. The fluid modeling staff includes professionals trained in environmental fluid dynamics, model makers, programmers, and laboratory and electronic technicians. The Air Pollution Training Institute (APTI) wind tunnel is available for calibration and response testing of wind measuring instruments.

The following pages depict the types of problems to which the wind tunnel may be applied. Clearly there are other applications.

For further information, contact:

Dr. William H. Snyder*
Physical Scientist
Model Development Branch

or

Dr. Douglas G. Fox*, Chief
Model Development Branch

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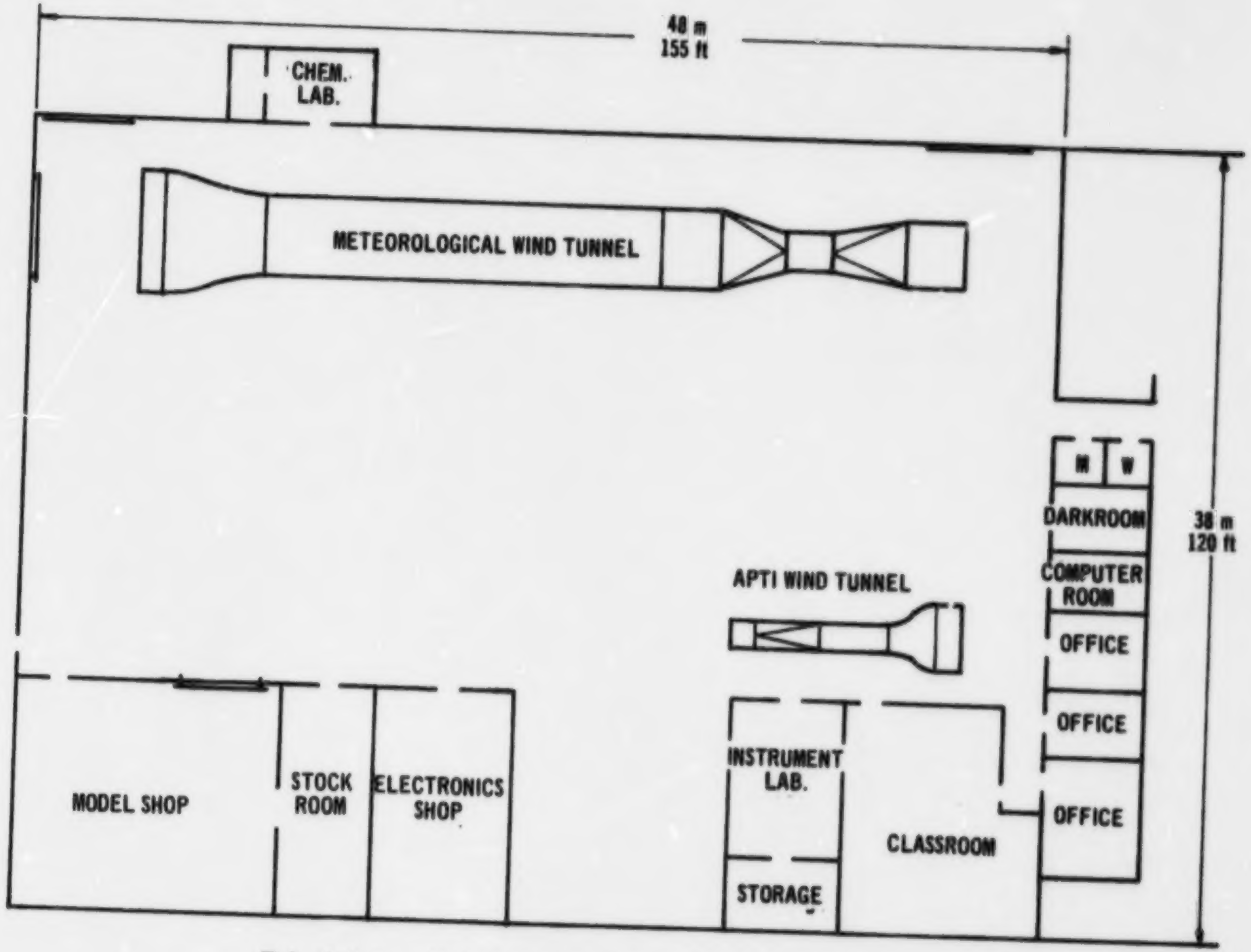
*On assignment from the National Oceanic and Atmospheric Administration U. S. Department of Commerce.

SPECIFICATIONS

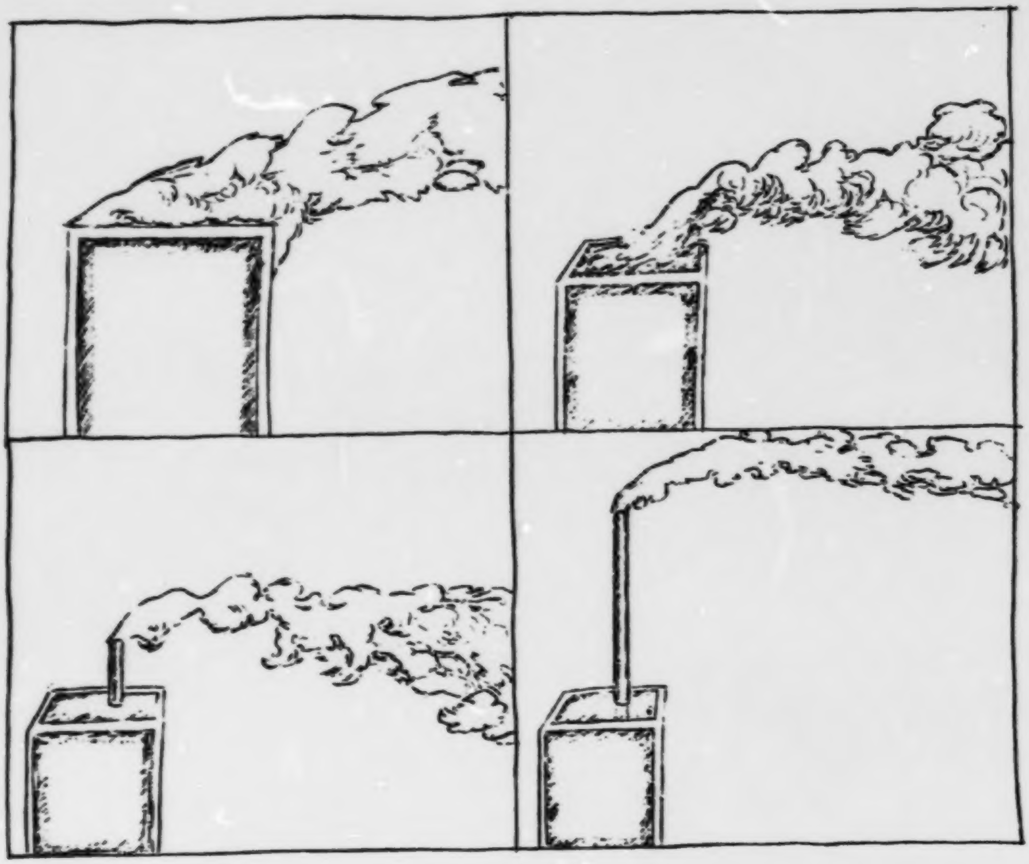
Characteristic	Meteorological Wind Tunnel	APTI Wind Tunnel
DIMENSIONS		
overall length	38 m (125 ft)	11 m (35 ft)
test section length	18 m (60 ft)	3 m (10 ft)
test section width	3.7 m (12 ft)	1 m (3 ft)
test section height	2.1 m (7 ft)	1 m (3 ft)
contraction ratio	2.8:1	4.5:1
WIND TUNNEL DRIVE		
Total Power	100 HP	25 HP
Type of Drive	72 in. axial fan	48 in. axial fan
Speed Control	AC motor/Eddy Current Coupler	DC motor/SCR control
SPEED	.5 to 8 mps (1.5 to 25 fps)	.3 to 21 mps (1 to 70 fps)

INSTRUMENTATION

- Instrument carriage in Meteorological Wind Tunnel providing 3 dimensional positioning of probes anywhere within test section with remote control and readout to within ± 1 mm.
- Flame ionization detectors for hydrocarbons
- Two channels of hot-wire anemometry with linearizers, filters, correlator, and integrator.
- Digital voltmeter
- Mini-computer with disc and magnetic tape drives, electrostatic printer/plotter and CRT.
- Smoke Generators

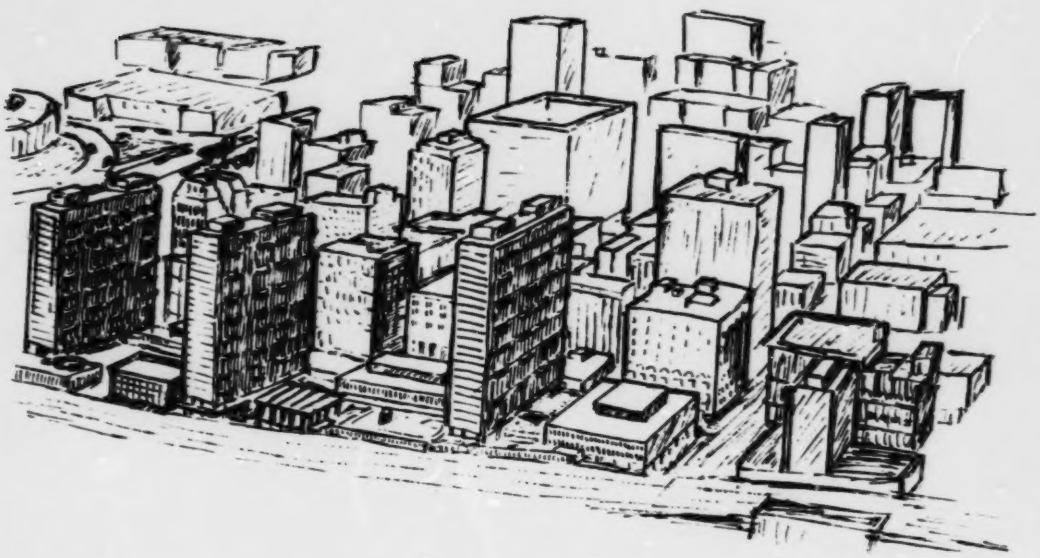

48 m
155 ft
CHEM.
LAB.
METEOROLOGICAL WIND TUNNEL
38 m
120 ft
M
W
DARKROOM
COMPUTER
ROOM
OFFICE
OFFICE
OFFICE
APTI WIND TUNNEL
INSTRUMENT
LAB.
CLASSROOM
STORAGE
MODEL SHOP
STOCK
ROOM
ELECTRONICS
SHOP

FLUID MODELING FACILITY
FLOOR PLAN



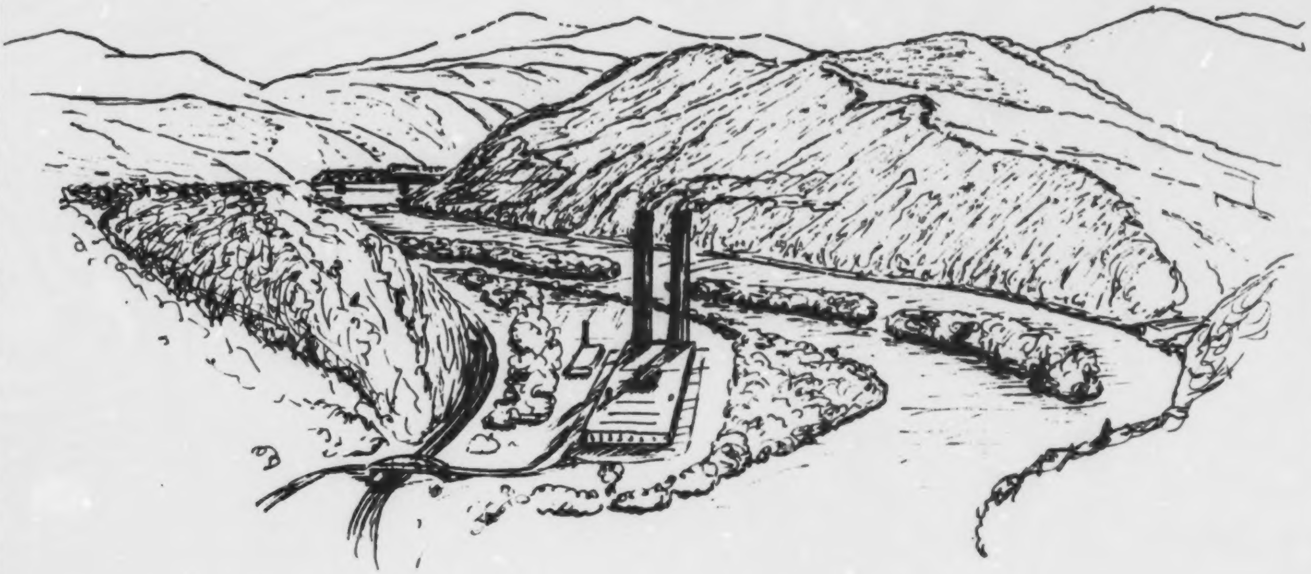
POLLUTANTS FROM STACKS

- BUILDING DOWNWASH
- STACK DOWNWASH
- LOCAL TOPOGRAPHICAL EFFECTS



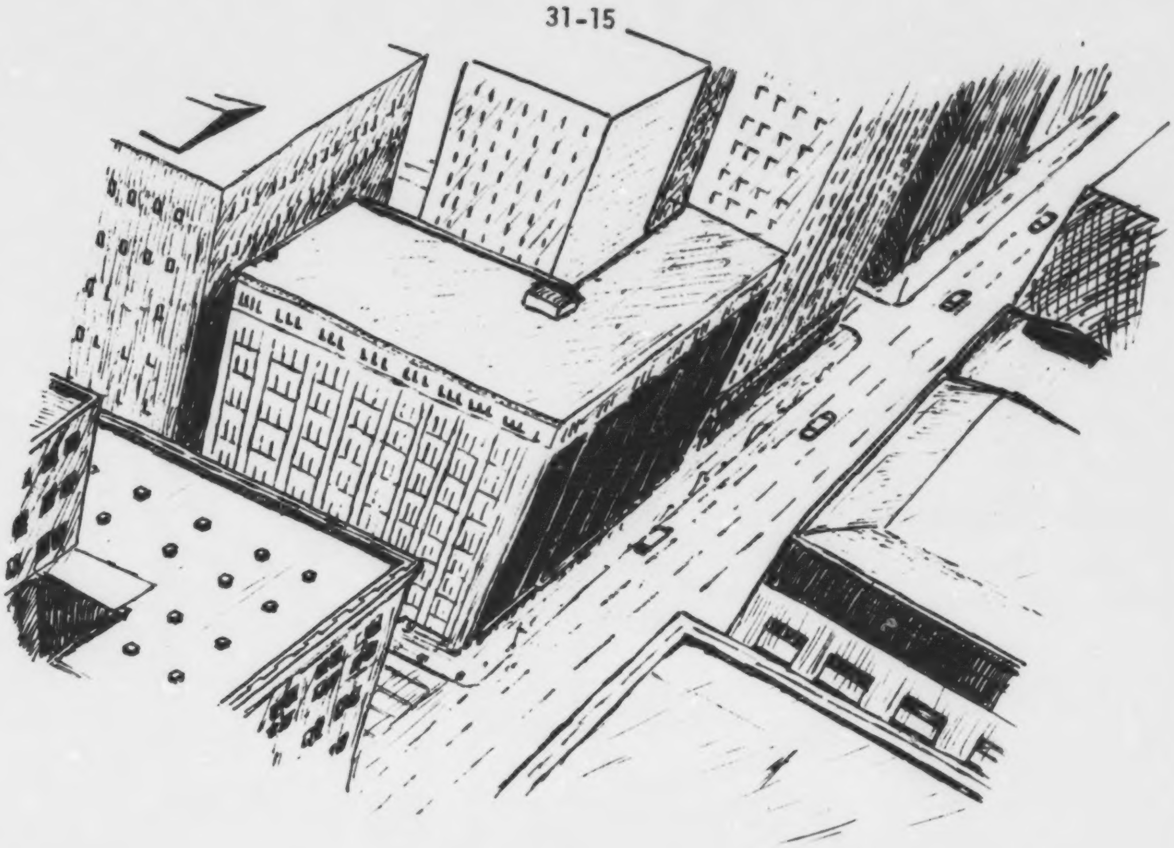
URBAN STRUCTURES

- SAMPLER POSITIONING AND PERFORMANCE
- SMALL SCALE DISPERSAL FROM TRAFFIC
- URBAN HEAT ISLAND
- EFFECTS OF NEW CONSTRUCTION
- URBAN ROUGHNESS
- WIND ENVIRONMENT



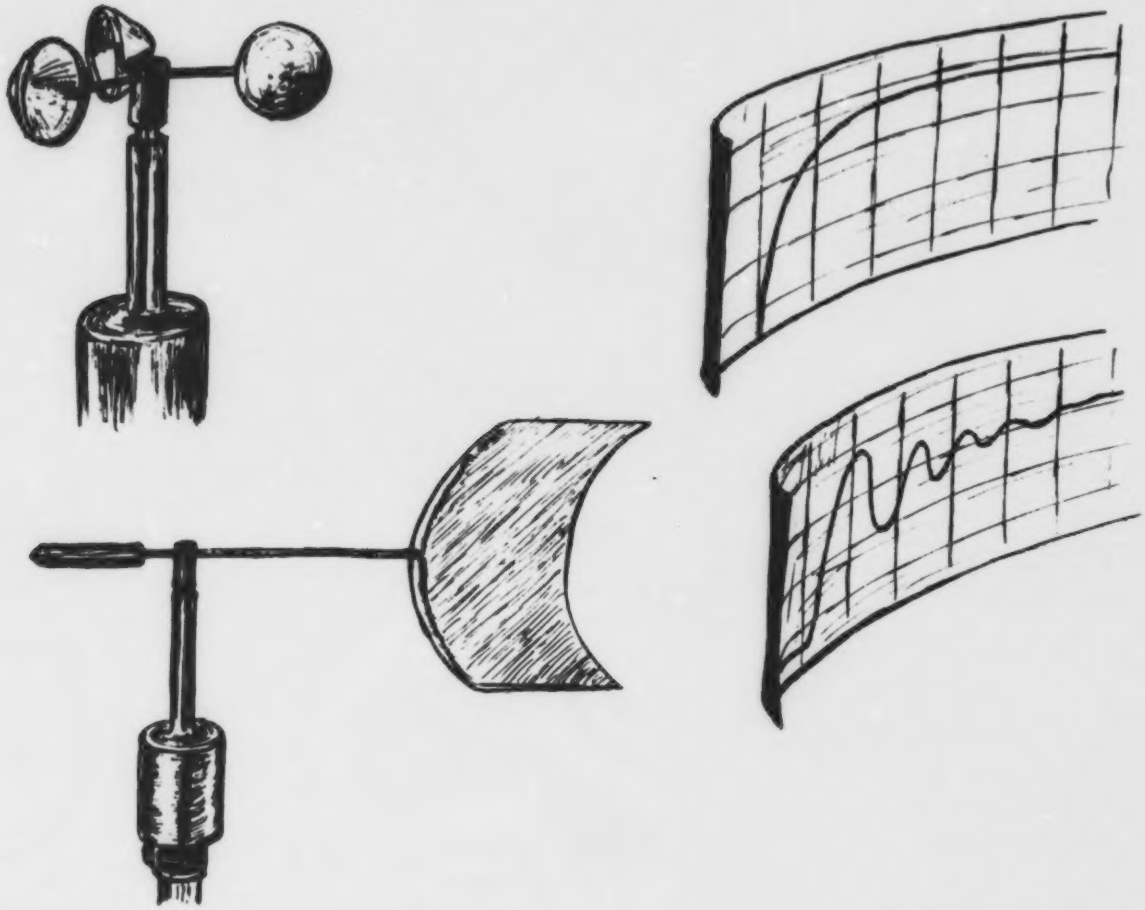
COMPLEX TOPOGRAPHY

- TOPOGRAPHICAL EFFECTS
- TERRAIN DOWNWASH
- FLOW DIVERSION AROUND HILLS
- PLUME RISE AND DIFFUSION
- MOUNTAIN-VALLEY WINDS



POLLUTION FROM AUTOMOBILES

- ELEVATED OR DEPRESSED HIGHWAYS
- STREET CANYONS
- "AIR-RIGHTS" STRUCTURES
- TUNNELS



WIND INSTRUMENT RESPONSE

- ANEMOMETER CALIBRATION
- DYNAMIC RESPONSE
- STALL SPEED
- TIME AND DISTANCE CONSTANTS

II. WIND TUNNEL TESTS OF DOWNWASH OF BUOYANT STACK GASES

Introduction

There is a "rule-of-thumb", evidently originating from wind tunnel tests by Sherlock and Lesher (1954), Strom (1955, 1956), Sherlock et al. (1958), Strom et al. (1957), and Halitsky (1962) which states that the speed of the effluent from a chimney must exceed one-and-one-half times the wind speed in order to avoid downwash of the effluent in the immediate lee of the stack.

The problem to be investigated here is: what is the effect of effluent buoyancy on this one-and-one-half times rule? It is not obvious upon first examination what effect the buoyancy will have. On one hand, the buoyancy forces will counteract the adverse pressure gradient in the lee of the stack (hereafter referred to as the flotational effect) so that the one-and-one-half times rule may be relaxed. On the other hand, the lighter stack gases will result in a lower effluent momentum, for a given effluent speed, so that the jet will be more easily bent-over by the wind (hereafter referred to as the momentum effect), and the one-and-one-half times rule may not be sufficient.

Theory

In early wind tunnel studies, the effluent was heated as high as 200°C in an attempt to simulate buoyancy. The results of

Sherlock et al. (1958) show a significant momentum effect, but a negligible flotation effect. They show that the behavior of the plume depends only upon the momentum ratio (or velocity ratio, provided that both velocities are reduced to equivalent velocities at a common temperature) and that flotational forces produced no measurable rise of the plume. Reexamining their work, however, it is evident that the densimetric Froude number was not properly modeled.

The Froude number represents the ratio of inertial to buoyancy forces in the effluent. It is:

$$Fr = \frac{W_o^2}{gD \, \Delta\rho/\rho}$$

where W_o = average effluent speed,

g = acceleration due to gravity,

D = internal stack diameter,

$\Delta\rho$ = difference in density between air and the effluent,

and ρ = effluent density.

A neutrally buoyant effluent would have an infinite Froude number. Buoyancy forces become important as the Froude number approaches unity, and the effluent Froude number of many industrial plants approaches unity. Although all the details are not given in the paper by Sherlock et al., it is evident that the effluent Froude number always exceeded 300. Thus, flotational effects were found to be negligible.

The Model

In the present study, dichlorodifluoro methane (freon 12) and helium were emitted from model stacks at low speeds in a wind tunnel to obtain a range of Froude numbers from 10^{-2} to 10^{3}. When freon (specific gravity :4.26) was used as the effluent, the stack was inverted in order to simulate a positive buoyancy. When helium (specific gravity :0.138) was used, the stack was placed in a normal (upright) position to simulate a positive buoyancy. A shadowgraph was created by directing a nearly parallel light beam across the stack onto a frosted glass background. Visual observations were made from the opposite side of the frosted glass screen. In a given run, the effluent was metered through a rotameter at a constant rate. The wind speed was varied and notes were made of the conditions at the point where downwash was incipient. Our definition of "incipient downwash" was when the effluent was observable approximately 50% of the time at a point at the stack surface one diameter below the top of the stack. This is a somewhat arbitrary definition, but it was used consistently throughout this set of experiments.

Results and Discussion

Figure 1 summarizes some results of the study. The ordinate is the ratio of effluent momentum to wind momentum at which downwash was incipient. For neutrally buoyant effluent, this would be simply the velocity ratio. Hence, if the flotation effect were negligible, this

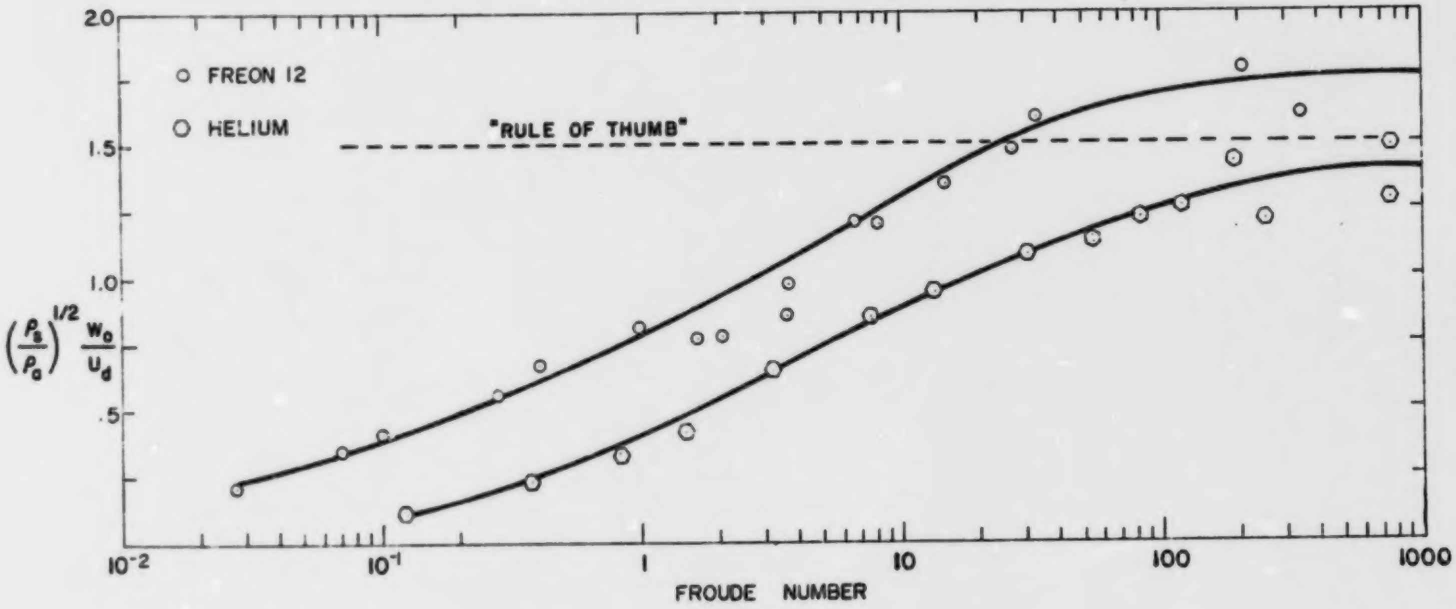


Fig. 1. Incipient Downwash

graph would be simply a horizontal straight line located at a momentum ratio of 1.5. It is seen that at large Froude numbers, the effluent speed must exceed nearly twice the wind speed in order to avoid downwash, according to our definition of incipient downwash. At very small Froude numbers, it is seen that the flotation effect is significant, i.e., because of its buoyancy, the effluent momentum needs to exceed only half the wind momentum to avoid downwash.

The separation between the two curves, one for helium, one for freon, is not fully understood. A possible explanation is the different visibility limits of the two gases. Some rather crude experimentation showed that only a 5% concentration of freon in air was required in order for the plume to be visible, whereas a 15% concentration of helium in air was required for detection. Hence, our choice of the definition of incipient downwash may not have been a good one, although it was the only means available at the time. Another possible explanation is the subtle distinction between the normal and inverted stack configurations, that is, the rate of entrainment of a light gas by a heavier gas (air by freon) may differ from the rate of entrainment of a heavy gas by a light gas (air by helium). In other words, the rate of entrainment may be a parameter in Figure 1. More quantitative experimentation using a flame ionization detector is under way to determine the cause of the separation.

III. WIND TUNNEL TESTS OF NEGATIVELY BUOYANT PLUMES

The Colorado State University conducted a wind tunnel study of negatively buoyant plumes under a grant from EPA (Hoot et al., 1973). Dense plumes, obtained by mixing dichlorodifluoro methane (freon 12) with air, were observed visually under a calm (wind tunnel) atmosphere, under a laminar crosswind, and in a turbulent boundary layer created using vortex generators a la Counihan (1969).

In a calm atmosphere, the maximum rise height, H, was found to be proportional to the Froude number:

$$H/D_o = 2.96 \text{ Fr},$$

where D_o = stack diameter

$\text{Fr} = W_o \sqrt{\rho_a} / \sqrt{g D_o (\rho_o - \rho_a)}$

W_o = effluent speed

ρ_o = effluent density

ρ_a = ambient density

and g = acceleration due to gravity.

Plumes in a laminar crosswind were correlated with the expression:

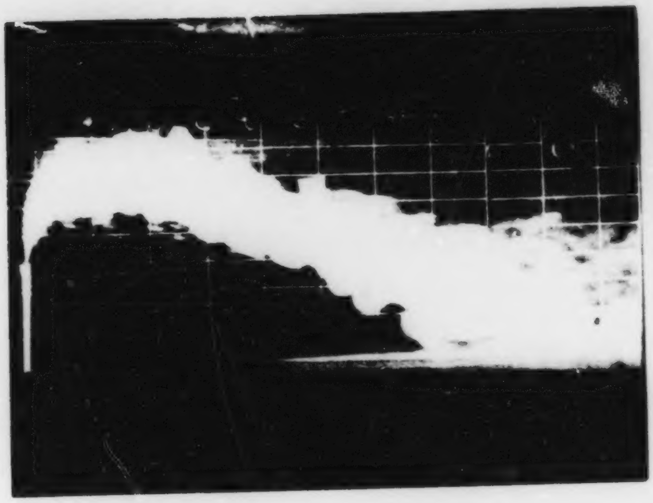
$$H/D_o = 1.32 \, R^{1/3} \, (SG)^{1/3} \, \text{Fr}^{2/3},$$

where $R = W_o/V$ (effluent speed/wind speed)

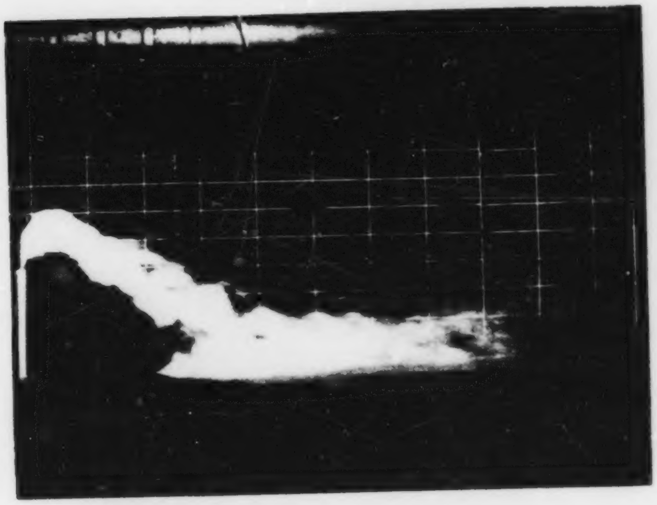
SG = effluent specific gravity (air = 1).

Figure 2, taken from Hoot et al. (1973), shows two typical smoke photographs. (The freon/air mixture was bubbled through titanium tetrachloride to produce a dense white smoke). Figure 3 shows the results of measurements of the horizontal distance from the stack base at which the plume touches the ground.

Once a negatively buoyant plume reaches the ground, it undergoes a more rapid lateral growth and a slower vertical growth than does a neutrally buoyant plume. This behavior is illustrated in Figures 4 and 5.



R=10.44, F_R=12.95, SG=2, U_o=7.50 ft/sec



R=5.14, F_R=5.60, SG=3, U_o=3.75 ft/sec

Fig. 2. Smoke Photographs

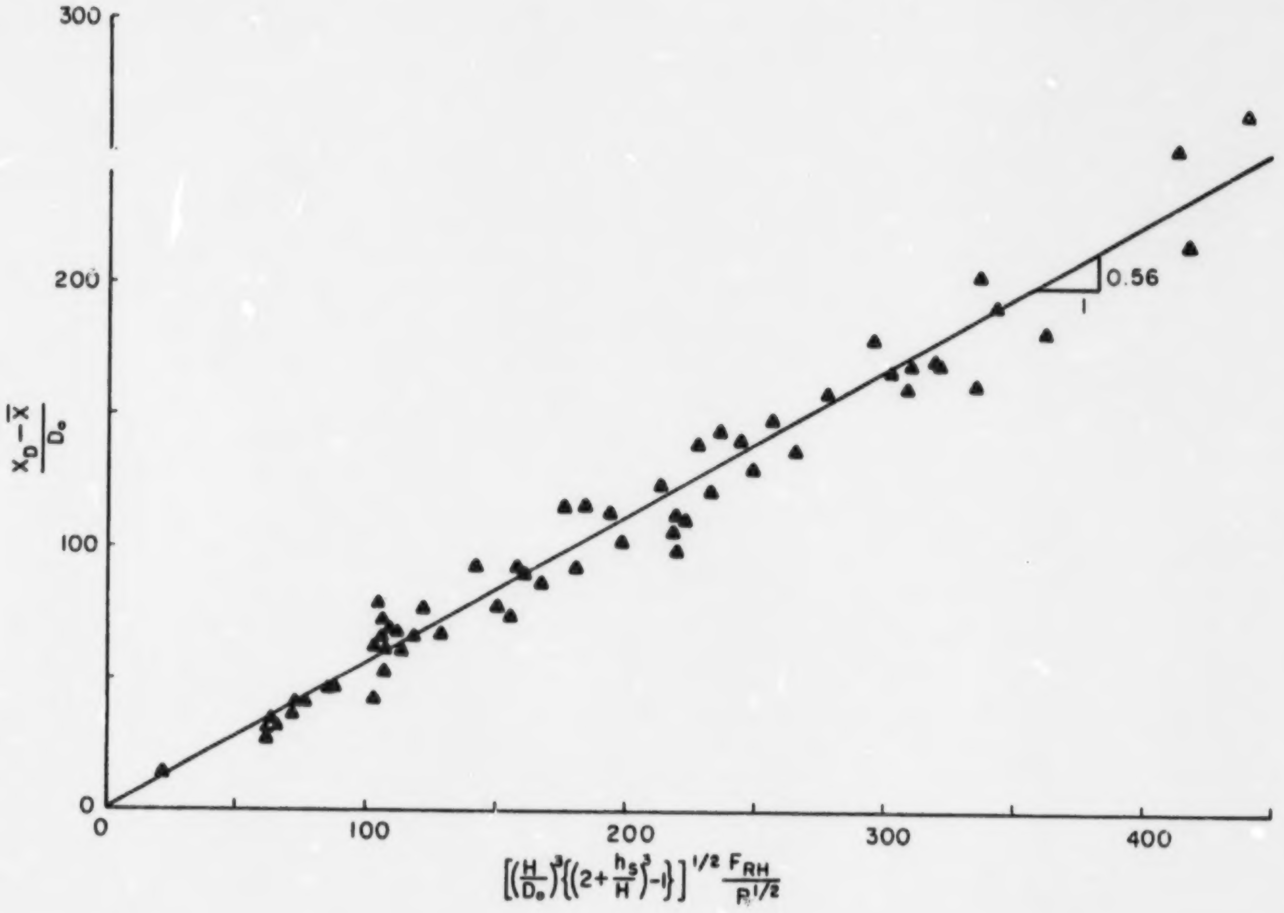


Fig. 3. Dimensionless "Touchdown" Distance vs. "Touchdown Parameter"

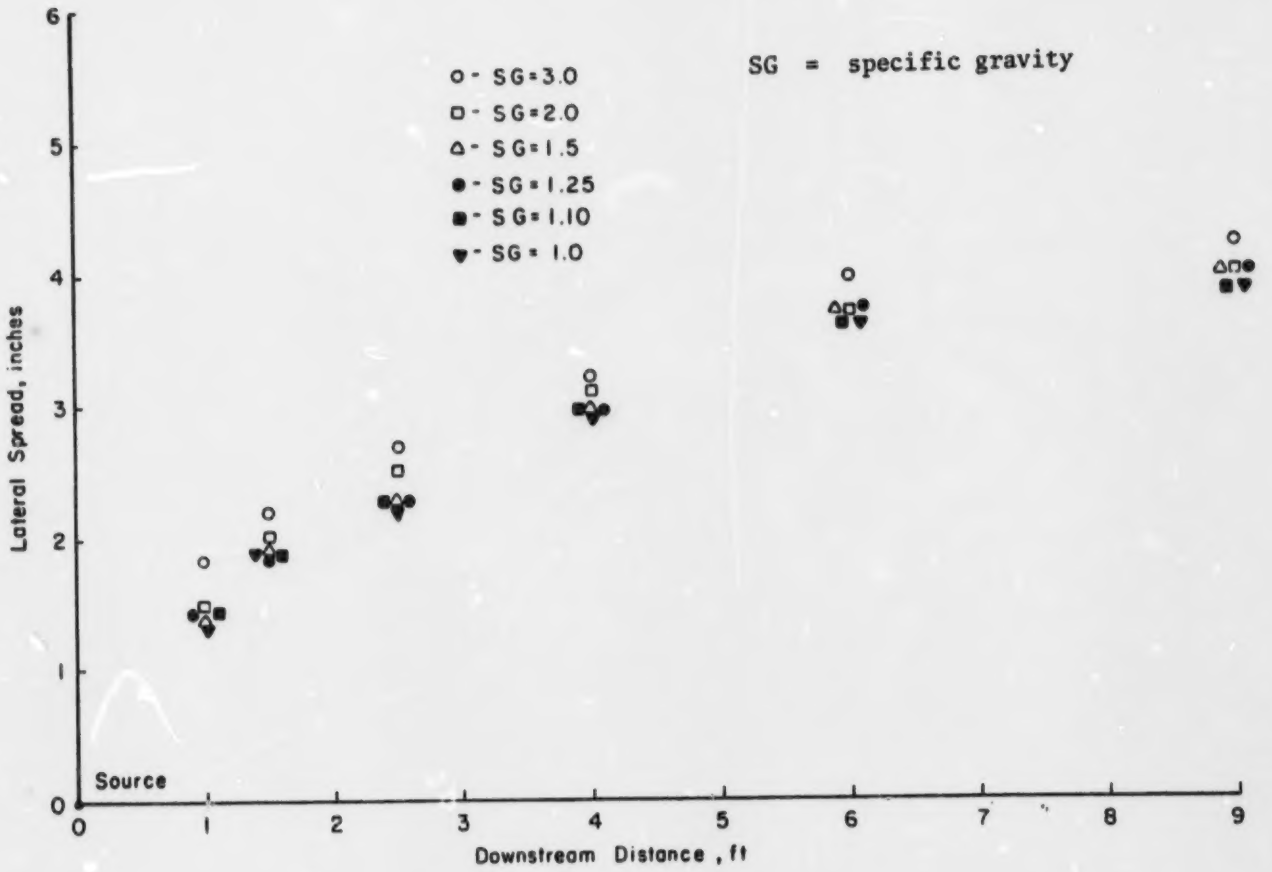


Fig. 4. Lateral Spread 10 Percent Concentration Neutral Stratification

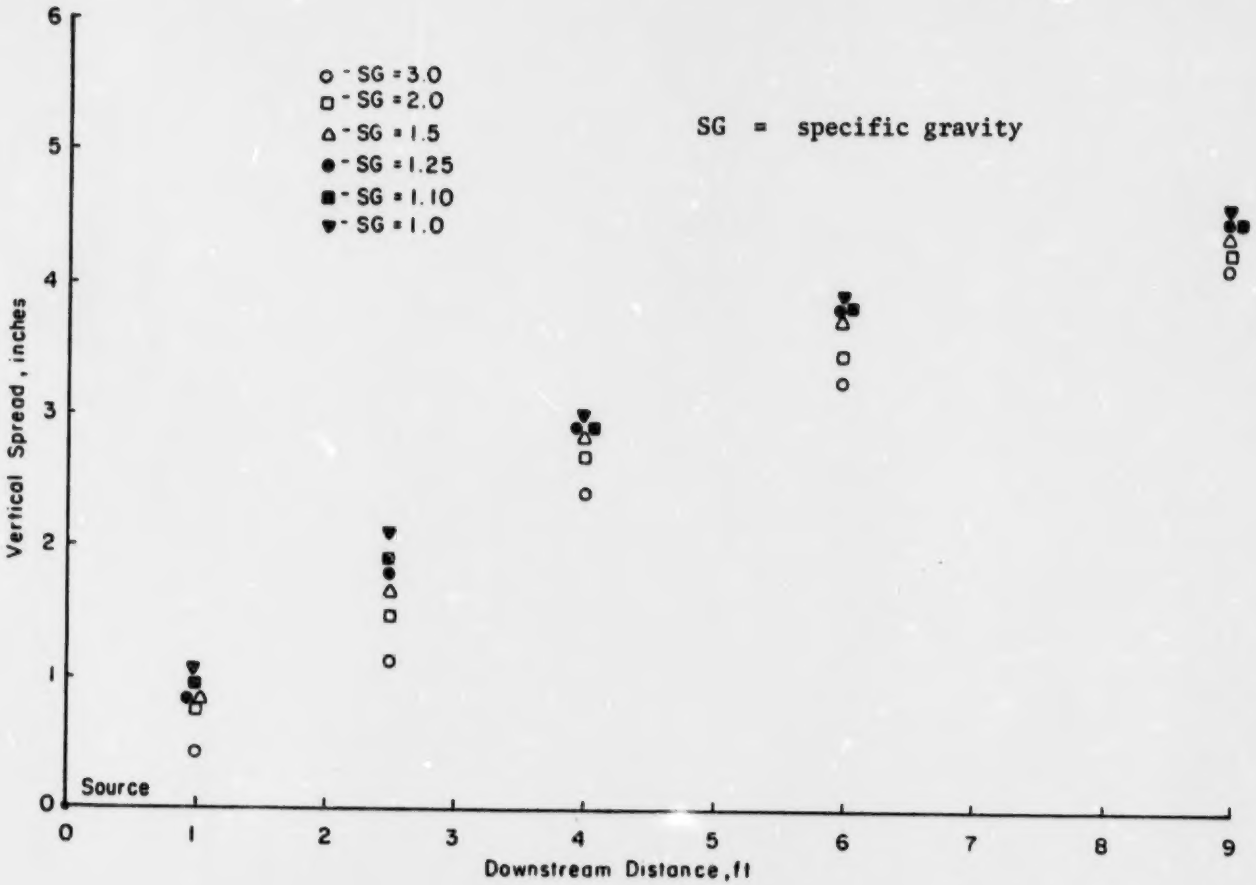


Fig. 5. Vertical Spread 10 Percent Concentration Neutral Stratification

IV. AIR POLLUTION TRANSPORT IN STREET CANYONS

The Los Alamos Scientific Laboratory (LASL) used a numerical model to calculate air pollution transport in street canyons under contract to EPA (Hotchkiss and Harlow, 1973). Their model employs solutions of the fully non-linear, three-dimensional Navier-Stokes equations coupled with transport equations for pollutant dispersal. The turbulence model consisted of a constant eddy diffusivity assumption. An analytical formulation was also developed for a two-dimensional street canyon.

The outputs from the model are displayed graphically in the form of perspective views. Figure 6 shows the steady velocity field established by the numerical model for a two-dimensional square street canyon. The stationary vortex structure, clearly observable in the figure, compares well with experimental data, although, because of a free-slip boundary condition, secondary vortices in the corners do not appear from the numerical model. Figure 7 shows the vortex structure established in a fully three-dimensional simulation of a street canyon in St. Louis, Missouri. Figure 8 shows the particle distribution resulting from a uniformly distributed area source at street level. Figures 9 and 10 show the comparisons between the numerical results and site measurements made by Ludwig and Dabbert (1972 The numerical results are scaled to match the experimental results at the lower left corner of the street canyon, but, even so, the structure of the concentration field and the gradients of concentration compare favorably.

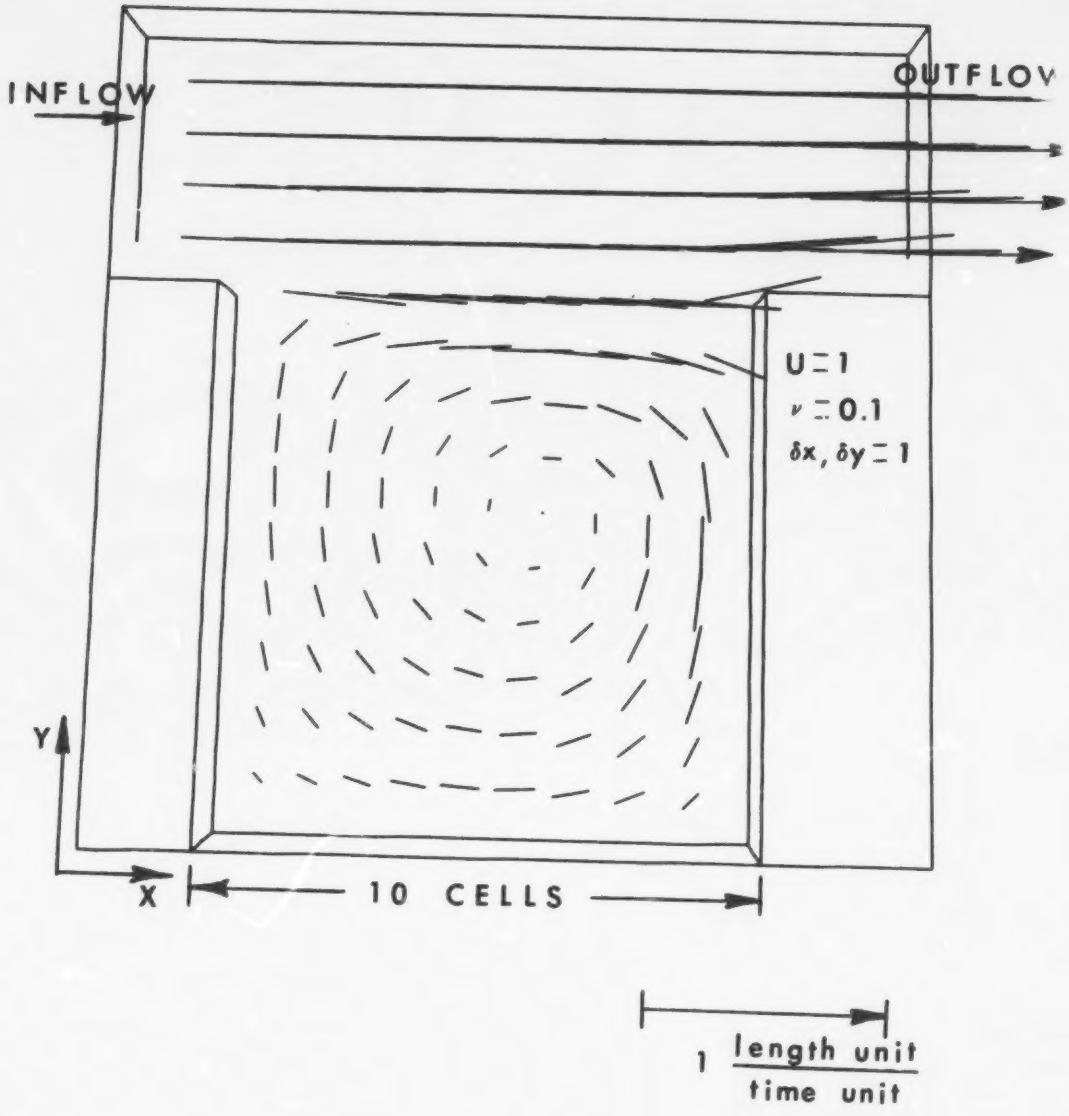

INFLOW
OUTFLOW
U = 1
ν = 0.1
δx, δy = 1
Y
X
10 CELLS
1 length unit / time unit

Fig. 6. Steady velocity field established in a two-dimensional square street canyon.

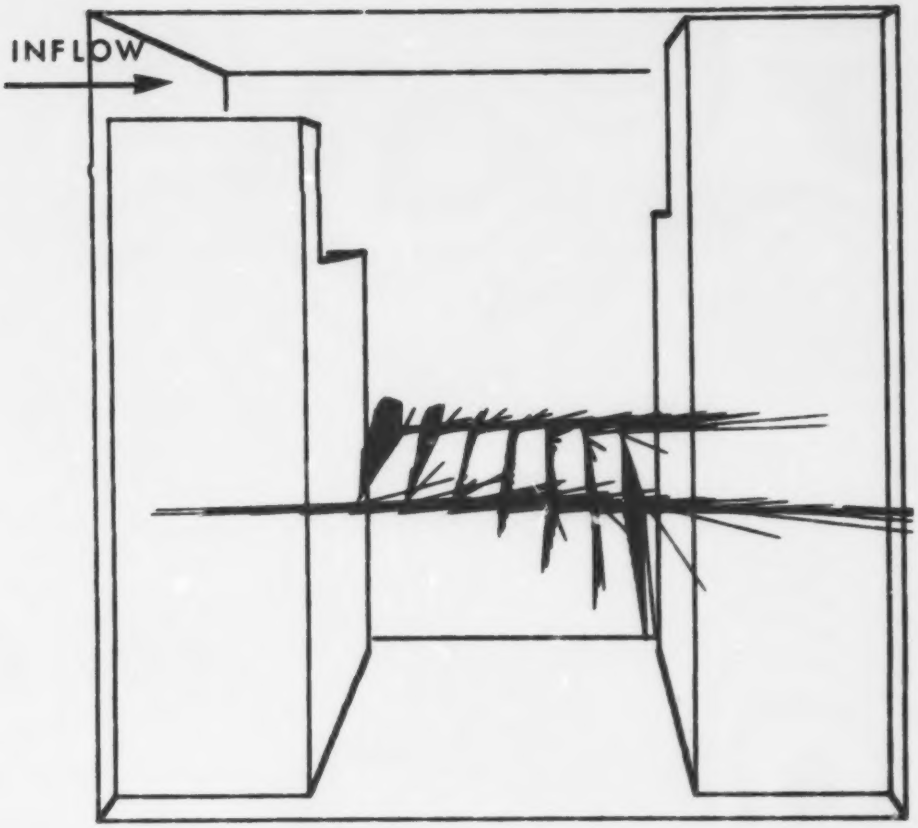


Fig. 7. Perspective view of velocity vectors in a plane perpendicular to the z axis at a distance of 65 feet from the origin.

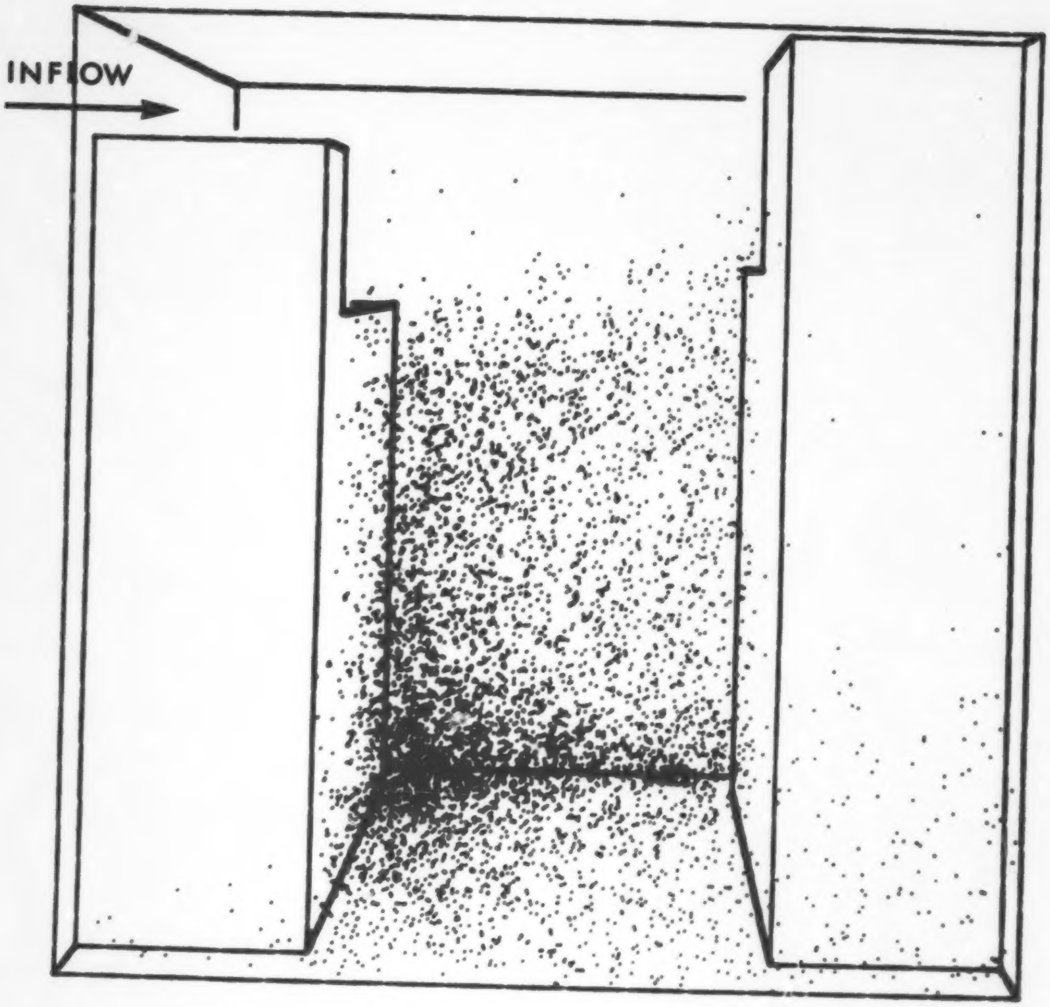


Fig. 8. Steady particular distribution in Broadway Street Canyon resulting from real sources on Broadway, Locust and Olive Streets.

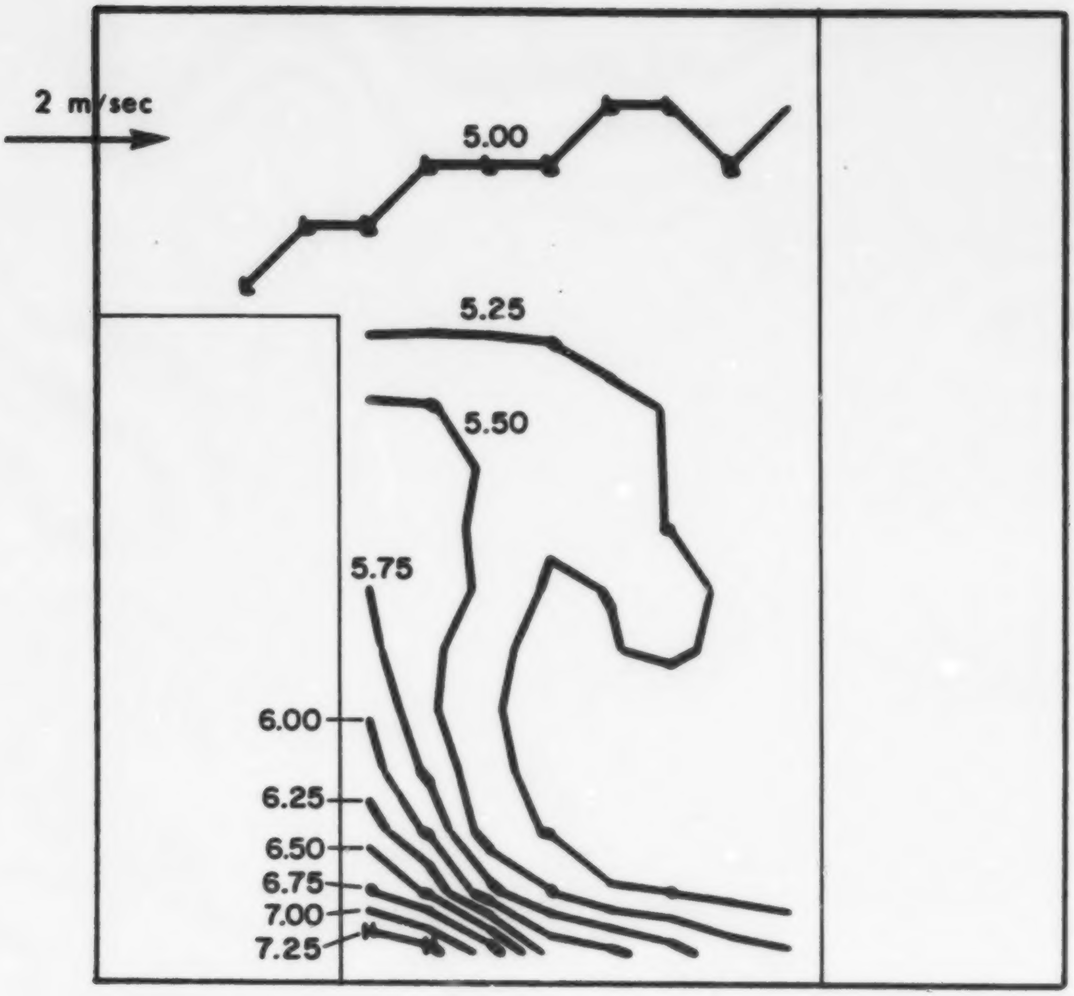


Fig. 9. Isopleths in a plane perpendicular to the x axis at a distance of 155 feet from the origin. This plot corresponds to the measuring station of Ludwig and Dabberdt. (Units in ppm of CO).

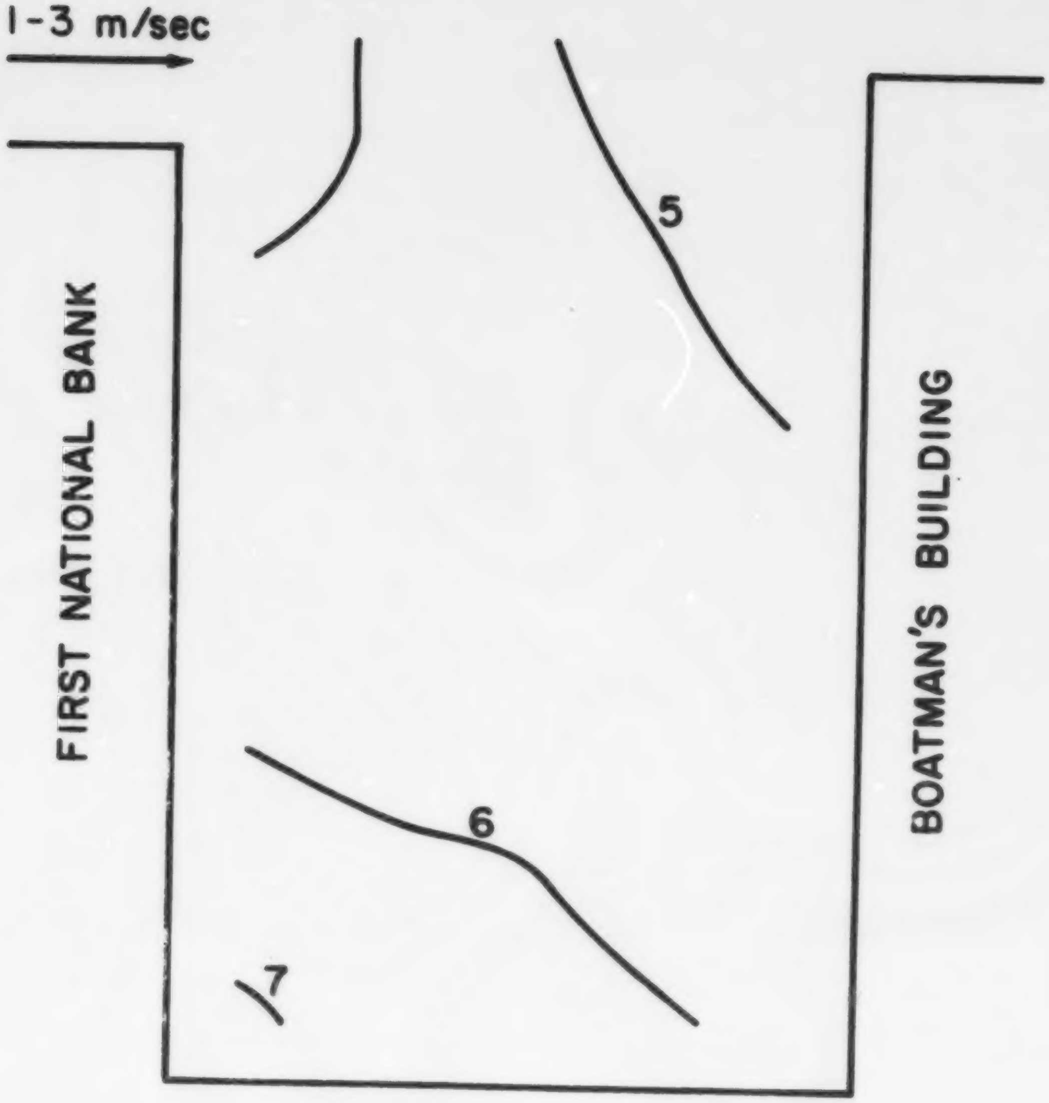

1-3 m/sec
FIRST NATIONAL BANK
BOATMAN'S BUILDING
5
6
7

Fig. 10. Distribution of CO concentration in Broadway Street Canyon (in ppm) measured by Ludwig and Dabberdt.

V. COOPERATIVE STUDY ON THE DISPERSION OF EFFLUENTS FROM THE CONEMAUGH POWER PLANT

A cooperative study between the French Meteorological Service (FMS) and the EPA Meteorology Laboratory (ML) was begun in 1970 to compare the results of field measurements of plume diffusion in complex topography with the results of measurements made in the water channel. ML made measurements of meteorological conditions, plant output, and concentration fields associated with the Conemaugh Power Plant in the vicinity of Johnstown, Pennsylvania, during the spring and fall of 1970 and 1971 (Schiermeier, 1972). From these data, days with near neutral stability were selected. Meteorological and plant output data for these selected days as well as topographical maps were supplied to the FMS.

FMS constructed a topographical model at a scale of 1:18000 and made some exploratory runs in their water channel using their colorimetric technique. This technique involves coating the surface of the model with pH-sensitive paint. Hydrochloric acid is released from model stacks and diffuses to ground level, thereby changing the color of the surface. Each color change, blue to green to yellow to orange to red, indicates a change of an order of magnitude in concentration. Thus, at the end of a run, ground level concentrations are vividly portrayed.

One of the wind directions studied in the exploratory runs corresponded roughly to field data which had been supplied. Comparisons between model and field results, however, were difficult for several reasons: 1) Most of the field samplers had been placed outside the range of the topographical model. 2) Helicopter measurements of ground level concentrations were accurate to only 1 pphm (27 $\mu g/m^3$). 3) The mean wind direction shifted somewhat during the field measurements. The few samplers located within the range of the model gave quite different results from those measured in the water channel, but, in view of the difficulties, the comparisons must be judged as inconclusive.

A later study allowed a more detailed comparison to be made. Meteorological parameters measured on October 28, 1970, over the Conemaugh area showed that the period from 1030 to 1230 hours could be considered as nearly ideal. The temperature profiles were very close to adiabatic and the mean wind profiles were unchanging. All the "bubblers" (SO_2 measuring instruments) were operating under/within the plume, and plant output conditions remained constant. Although the time of operation as well as the averaging time varied slightly from station to station, average values were calculated for the approximate 2-hour period. According to the FMS, the corresponding averaging time in the model was 3 hours, 45 minutes.

Figure 11 shows the isoconcentration map from the FMS. Unfortunately, it was not possible to duplicate here the multiple colors as in the original. The bubbler locations are indicated by dots with arrows, except for G27 which is just off the boundary of the model. The table below shows the comparative results.

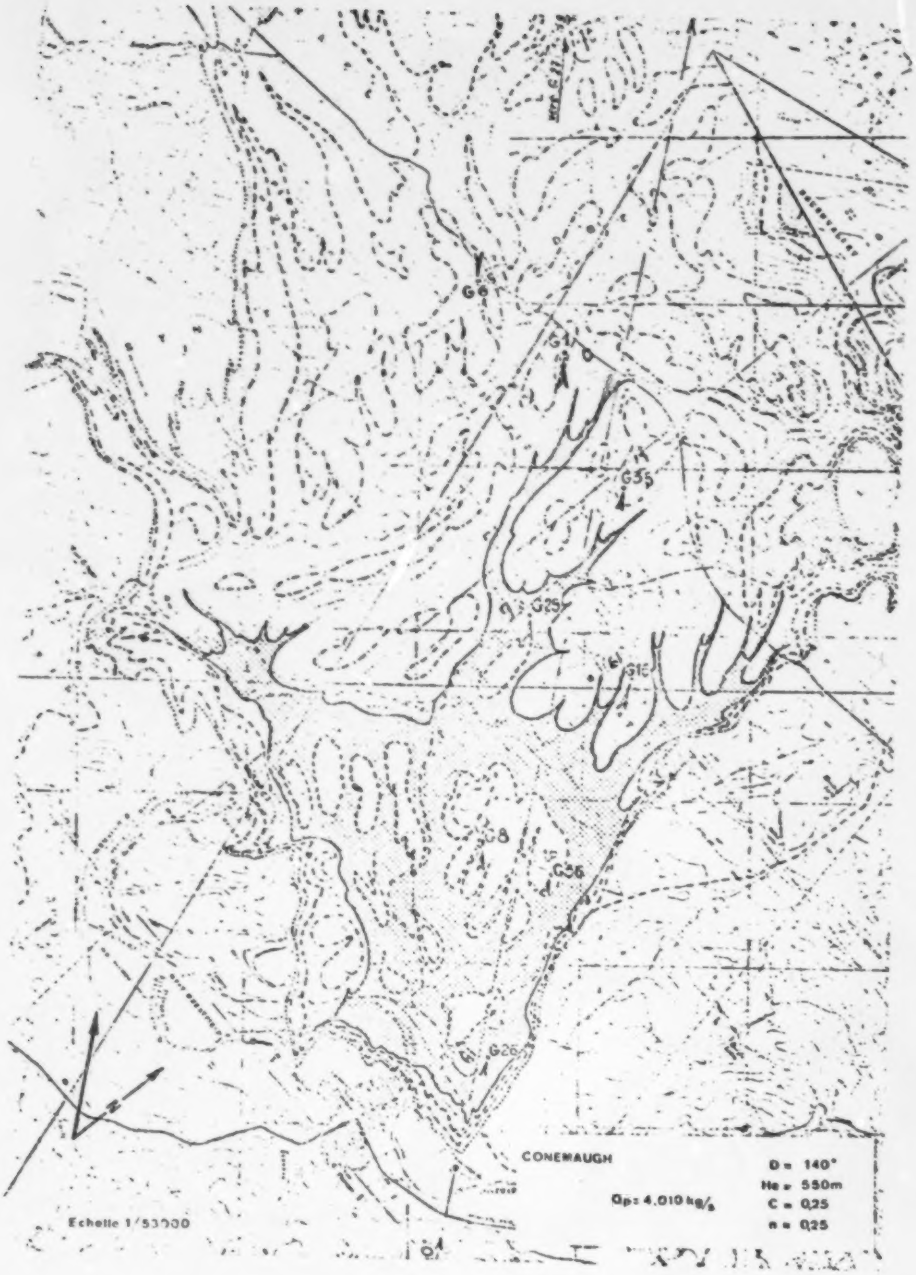

G6
G17
G35
G25
G15
G8
G36
G26
CONEMAUGH
D = 140°
He = 550m
Qp: 4,010 kg/s
C = 0,25
n = 0,25
Echelle 1/53000

Fig. 11. Isoconcentration Map - Conemaugh Plume

Bubbler Number	Bubbler Concentration ($\mu g/m^3$)	Model Concentration ($\mu g/m^3$)
G26	81	$x > 100$
G36	20	$10 < x < 100$
G8	101	$10 < x < 100$
G25	95	$x > 100$
G16	61	$10 < x < 100$
G35	14	$1 < x < 10$
[illegible]6	59	$1 < x < 10$
[illegible]	0	$1 < x < 10$
G27	40	$x < 100$

Strictly speaking, only 3 of the 9 measurements are within the bounds predicted by the model. Allowing for the inaccuracies in the bubbler readings of ± 1 pphm (± 27 $\mu g/m^3$), 8 of the 9 measurements are within the bounds. Slight changes in wind direction can also change the concentrations drastically. For example, a 10° rotation of the wind might result in concentration changes at G36 from $x > 100$ to $x = 0$ $\mu g/m^3$.

In summary, whereas the comparisons shown here do not prove nor disprove the validity of the water channel simulation technique, they do lend plausible support.

The French company Securipol has constructed a large water channel, with provisions for producing stratified flows, at Evian to study similar types of problems using the colorimetric technique of the FMS. Securipol is anxious to continue the Conemaugh study, particularly under stratified conditions. ML is presently preparing the data for transmittal to Securipol.

VI. STRATIFIED TOWING TANK SIMULATION OF PLUME DISPERSION OVER COMPLEX TERRAIN

Flow Research, Inc., under contract to EPA, conducted a towing tank study of the dispersion of a plume from an elevated source upwind of an idealized mountain (Gaussian-shaped saddle) under neutral and stably stratified flow conditions (Lin et al., 1974). The topography and stack location are shown in Figures 12 and 13. The model was inverted and towed through the tank, with a concentrated salt solution as the effluent. Linear density profiles were created by filling the tank with layered mixtures of salt water, each layer slightly different from the adjacent layer. Dyes and shadowgraphs were used for flow visualization. Temperature was used as a tracer for quantitative concentration measurements.

A close examination of Figure 14 reveals many qualitative results of the study. Figures 15, 16, and 17 show plots of plume trajectories and horizontal and vertical plume spreading. The nomenclature in the figures is:

$$F_D = \frac{W_s}{\sqrt{gD \frac{\Delta\rho}{\rho_s}}}$$, stack Froude number,

$$F_h = \frac{U_\infty}{Nh}$$, internal Froude number based on ridge height,

$$F_H = \frac{U_\infty}{NH}$$, internal Froude number based on stack height,

$$K = \frac{W_s}{U_\infty} \quad \text{, velocity ratio,}$$

$$N = \frac{1}{2\pi} \sqrt{\frac{g}{\rho_a} \frac{d\bar{\rho}}{dz}} \quad \text{, Brunt-Vaisala frequency,}$$

and $$R_D = \frac{W_s D}{\nu} \quad \text{, Reynolds number,}$$

where W_s = effluent speed,

g = acceleration due to gravity,

D = stack diameter,

$\Delta\rho = \rho_s - \rho_a$

ρ_s = effluent density,

ρ_a = ambient density at stack top,

h = mountain peak height,

U_∞ = free stream velocity,

H = stack height,

and ν = kinematic viscosity.

The numerical values assigned to the most important dimensionless parameters were chosen to be typical of industrial plants in the western United States under reasonably stable meteorological conditions.

Some highlights of the study include: 1) the presence of the terrain within the stably stratified flow creates an upstream blocking situation. As a result, plume rise and spreading are increased because the local velocity ratio, W_s/U_a, is increased. In one instance, a significant amount of pollutant was trapped in the blocked region just upstream and below the mountain ridge.

2) Because the vertical motion is inhibited by the stable stratification, the plume tends to flow around rather than over the ridge, thus the lateral plume spread is greatly enhanced.

3) The mean and fluctuating concentrations are larger at stations on the mountain ridge than at other surface stations.

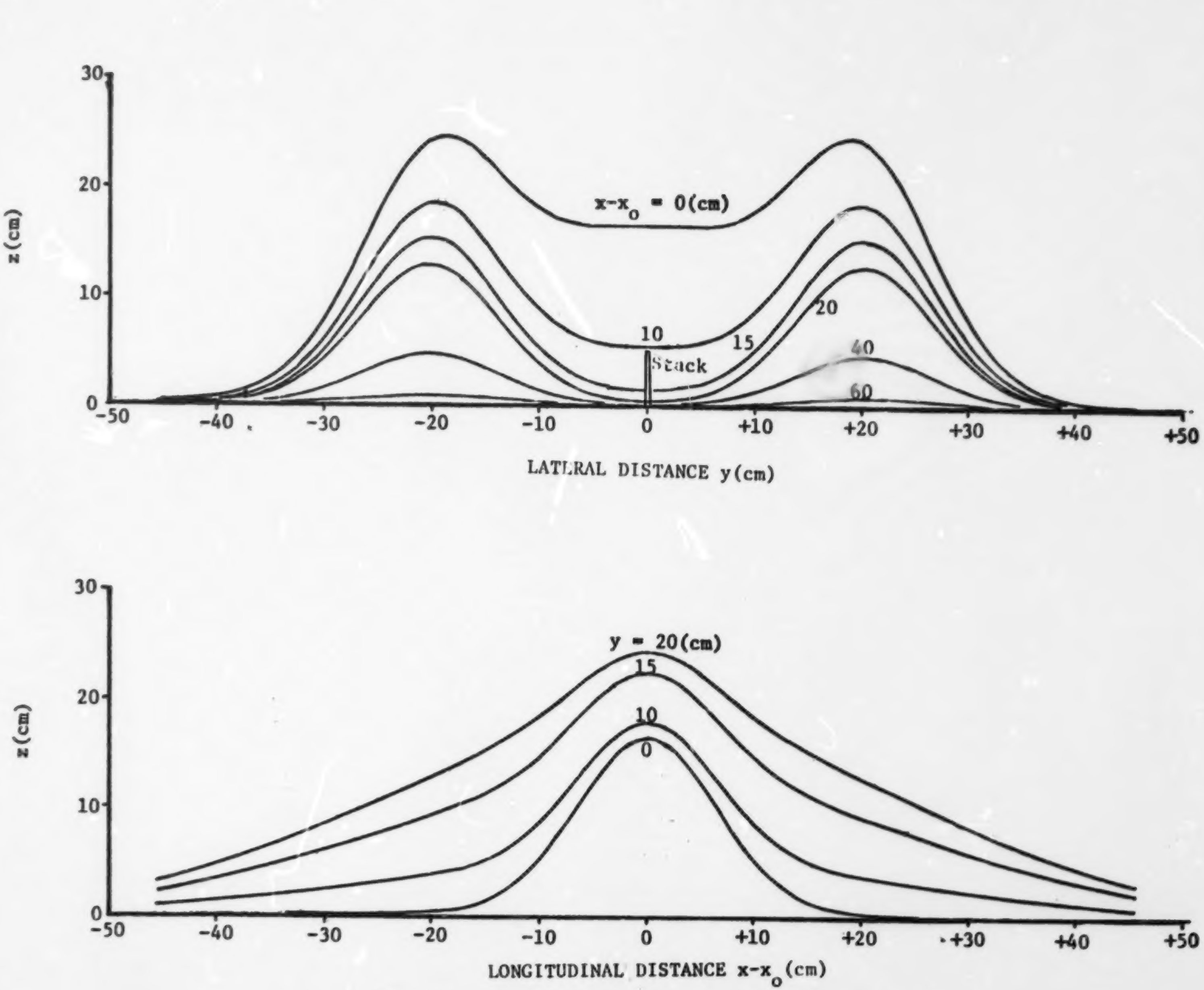


Fig. 12. Cross-sectional Views of the Terrain Model.

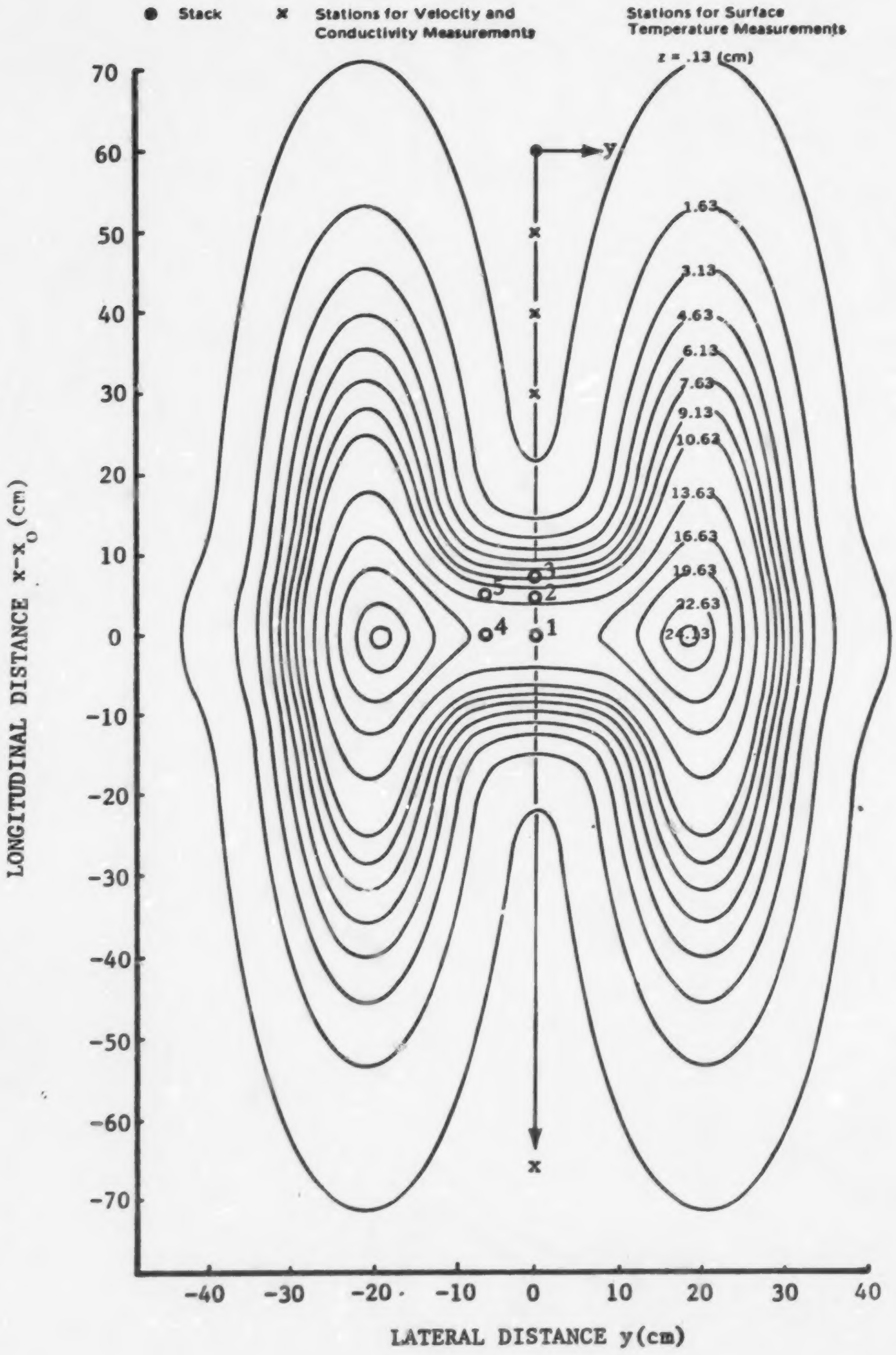

● Stack
x Stations for Velocity and Conductivity Measurements
Stations for Surface Temperature Measurements
z = .13 (cm)
1.63
3.13
4.63
6.13
7.63
9.13
10.63
13.63
16.63
19.63
22.63
24.13
1
2
3
4
5
y
x
70
60
50
40
30
20
10
0
-10
-20
-30
-40
-50
-60
-70
-40
-30
-20
-10
0
10
20
30
40
LONGITUDINAL DISTANCE x-x_0 (cm)
LATERAL DISTANCE y(cm)

Fig. 13. A Contour Map of the Terrain Model

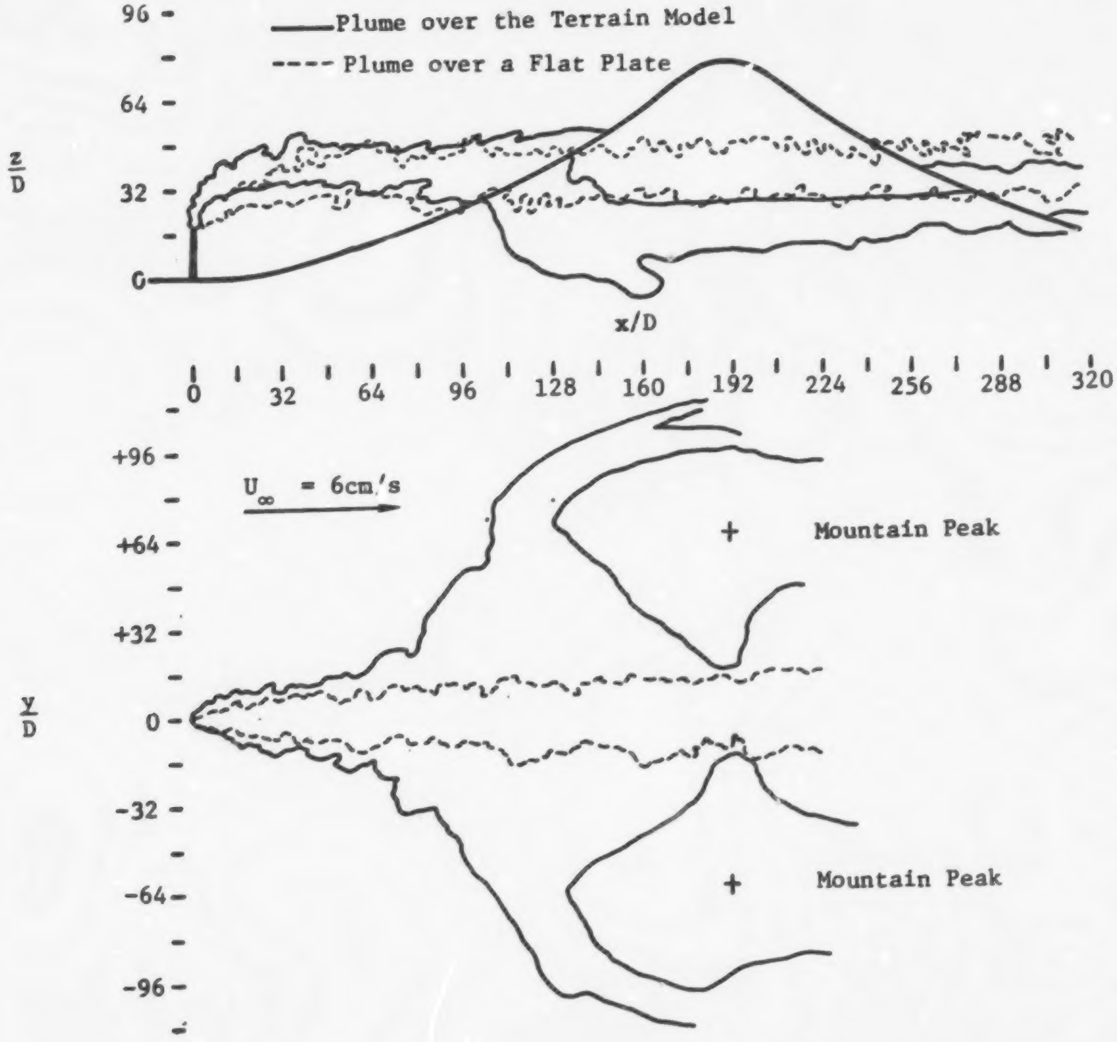


Fig. 14. Vertical and Lateral Spreads of Plumes In Stratified Flows over a Flate Plate and the Terrain Model. $F_D = 3.16$, $F_h = 2.64$, $F_H = 6.22$, $K = 3.4$, and $R_D = 530$.

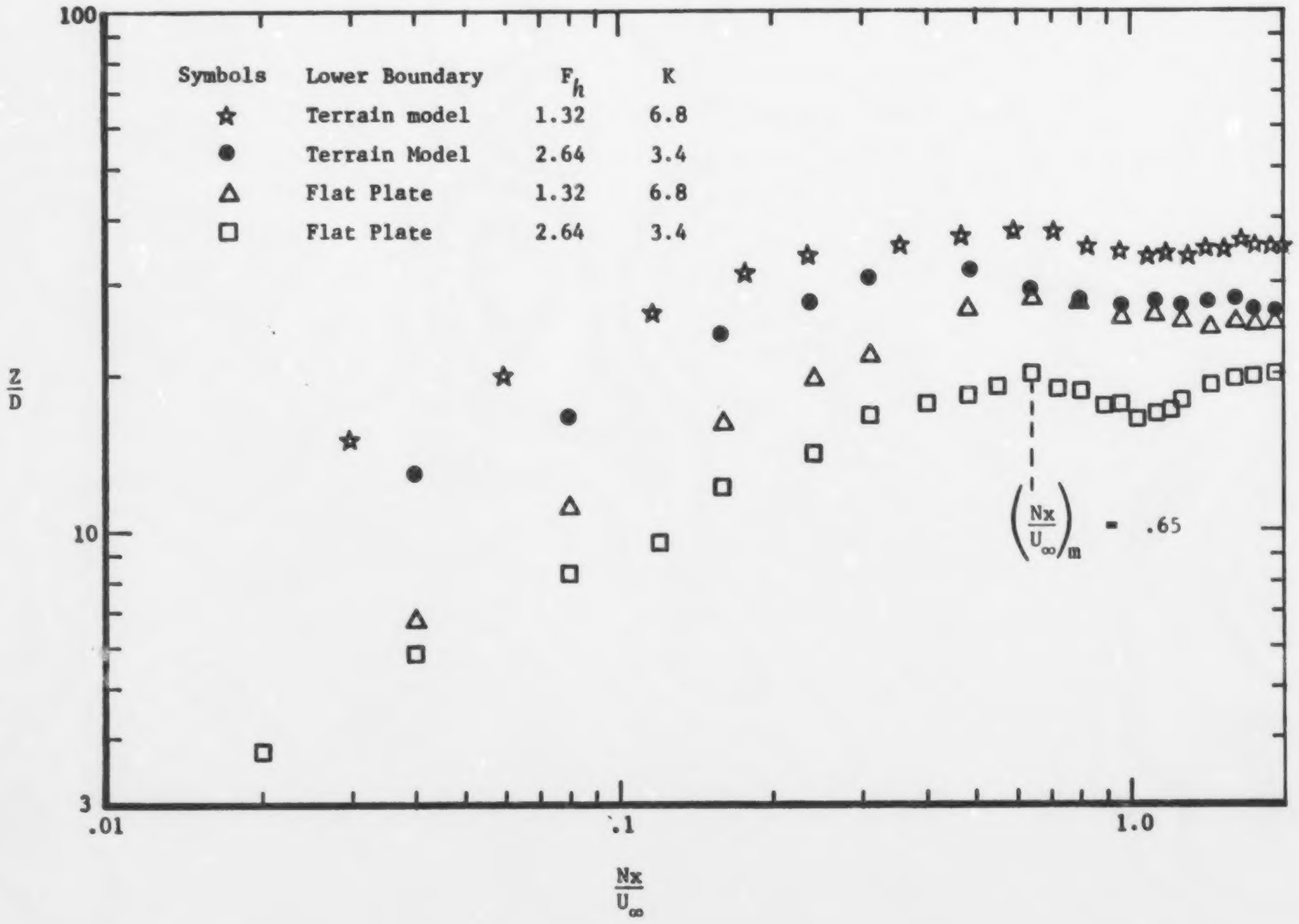


Fig. 15. Terrain Effects on the Rise of Plumes (F_D = 3.16) in Stably Stratified Flows.

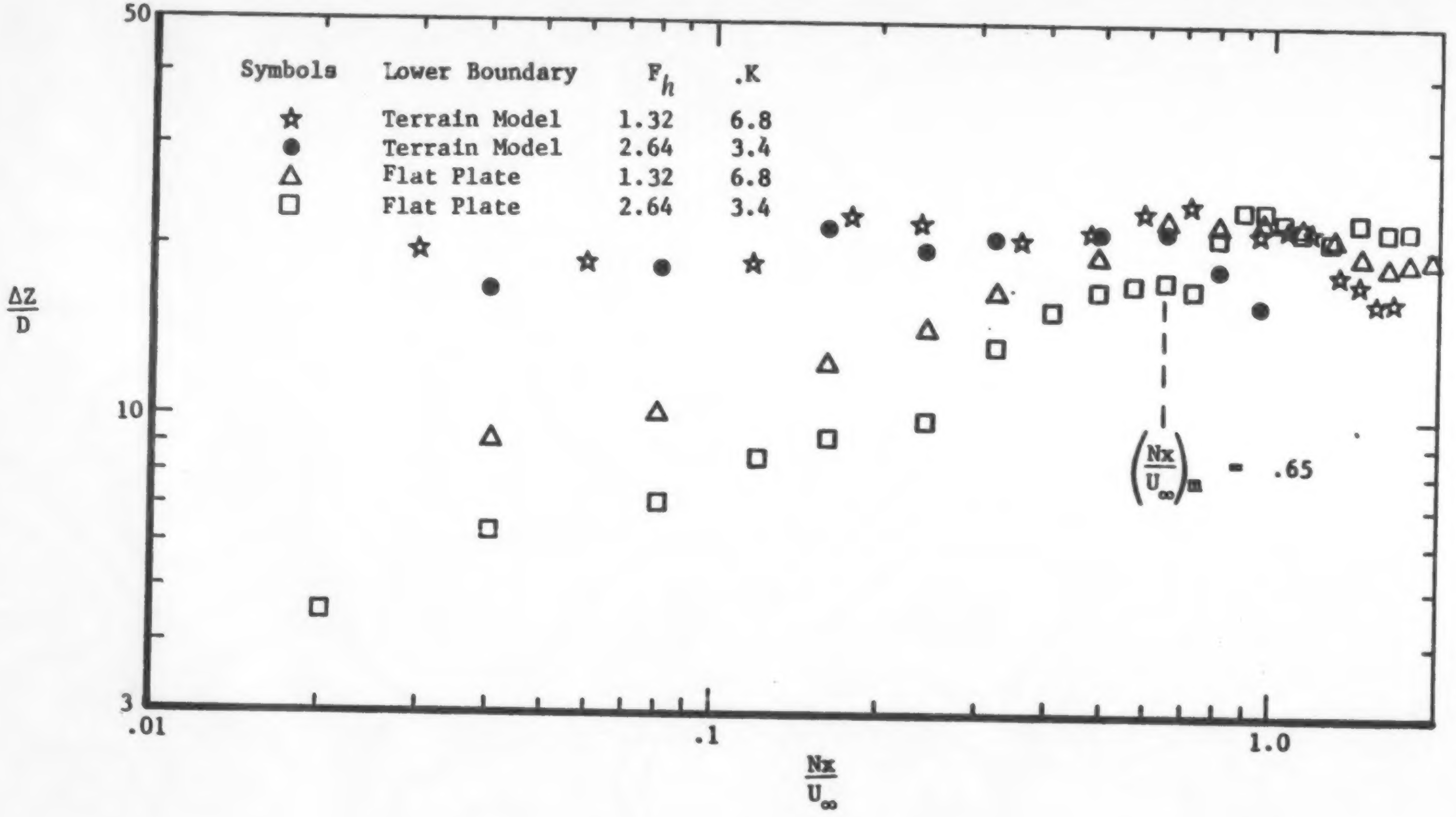


Fig. 16. Terrain Effects on the Vertical Spreads of Plumes (F_D = 3.16) in Stably Stratified Flows.

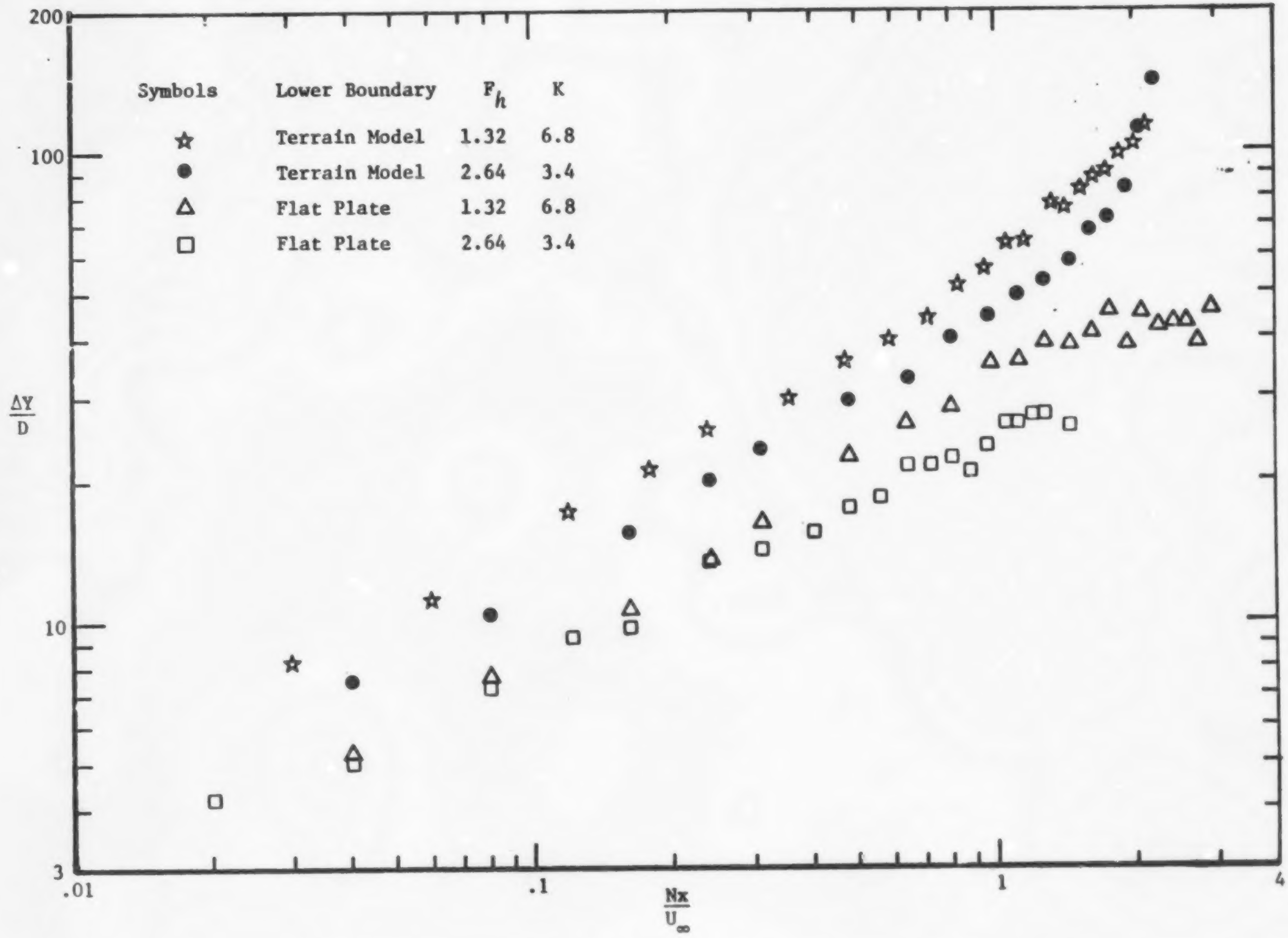


Fig. 17. Terrain Effects on the Lateral Spread of Plumes (F_D = 3.16) in Stably Stratified Flows.

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Chapter 32

A QUANTITATIVE APPROACH TO CLIMATOLOGICAL SITE STUDY

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

I - INTRODUCTION

The purpose of this paper is to show how we can approach the problem of predicting the levels of pollution created by a conventional power plant before it is planted. We choose to study the site of ARAMON where E.D.F. plans to build a power plant of two 700 MW groups with a 250 meter stack.

ARAMON is a little village situated in the RHONE valley, between AVIGNON, the city of the Popes, and TARASCON, the town of TARTARIN (fig. 1).

The site of the future power plant is characterized as follows :

- First, a rather complex topography, which, however doesn't exceed 200 meters.

- Second, frequent strong winds. The Mistral, especially, blows about 100 days a year (fig. 2).

The numerical air pollution dispersion model used is based on LUCAS's formula for plume rise and PASQUILL's formula for dispersion. We simulate the functionning of the power plant during a period of one or several years. Therefore, we use trihourly meteorological data -wind speed and direction and cloudiness- given by a national weather station (the nearest weather stations are : ORANGE, 30 km at North of ARAMON, and NIMES, 20 km at West of ARAMON). The 3 hours concentration are deduced from PASQUILL's formula with using a rate of decrease -from 10 minute to 3 hours sampling time - equal to 0.4 .

The use of such a model sets three kinds of problems :

1) Problems related to the topography, that is to say the influence of the topography on the local wind pattern.

.../...

2) Problems related to the meteorological data : the model requires the previous knowledge of a certain number of meteorological parameters which characterize the structure of the local atmospheric boundary layer.

3) The problem of adapting PASQUILL's curves to the characteristics of the site, and studying the influence of the sampling time on the rate of dispersion. Particularly, we intend to adjust the 3 hours to 10 minutes concentration ratio according to wind structure and atmospheric stability.

II - INFLUENCE OF TOPOGRAPHY

We studied the general wind pattern with the aid of a water tunnel (fig. 3). The horizontal scale used was 1/10000 and the vertical one was 1/3000. The velocity measurements were taken by hot wires.

Therefore, we studied different wind velocities and directions and measured the velocity field at different levels.

For North wind, we observed at 10 meters a channeling effect in the flow pattern, but none on the site of the power plant ; at 85 meters a slight effect still remained, though it disappeared at 220 meters (fig. 4).

For South East wind, we observed the strong effect of the central hill on the flow pattern at 10 m and 85 m levels, and an attenuation at 220 m. (Fig. 5).

III - STRUCTURE OF LOCAL ATMOSPHERIC BOUNDARY LAYER

We started erecting four anemometric stations between AVIGNON and ARLES. The stations are equipped with skyvane, wind sensors at the 11 meter level.

We next carried out two series of field tests 3 weeks in November 1973 and three others in March 1974 :

All the measurements were taken from a base situated on the left bank of the RHONE facing the building site of the future power plant -which is a few kilometers avay from ARAMON- (fig. 6).

For pressure, temperature and humidity measurements, we used the equipment commonly used by National Weather Service : a measural radiosonde, an Eider receiver station -the data were recorded on a perforated type-.

We used two theodolites to track pilot balloons. These theodolites were equipped with a numerical coding system. Every five seconds, the values were automatically recorded on a cassette.

All these data are not completely interpreted. This interpretation is now being carried on for the following purposes :

1) To try to find out a correlation between the meteorological situation observed on the site of ARAMON and the situation observed in the neighbouring permanent weather stations.

2) To point out a certain number of characteristic wind profiles, related with the wind speed and the atmospheric stability.

3) To point out an evolution pattern between two instantaneous meteorological situations, observed for instance at 1 a.m. and 1 p.m.

.../...

4) To study the mechanism of the formation and the evolution of temperature inversions.

IV - TURBULENCE STRUCTURE AND INFLUENCE OF THE SAMPLING TIME ON THE EVALUATION OF DISPERSION PARAMETERS

We intend to adapt PASQUILL's curves considering turbulent characteristics of the power plant, and to study the influence of the non stationnary character of the atmospheric turbulence over the rates of dispersion, in order to rectify the ratio of 3 h to 10 mn concentrations, which in our model is assumed to be constant and equal to 0.4 .

During the field tests, mentionned earlier we used a 35 meter tower. Elements to be measured were : wind speed and direction, fluctuations of wind speed -in the three components- , azimuth and elevation angles, and temperature. Selection of heights at which measurements were taken was based on a logarithmic spacing. The individual instruments under consideration are shown in table 1 .

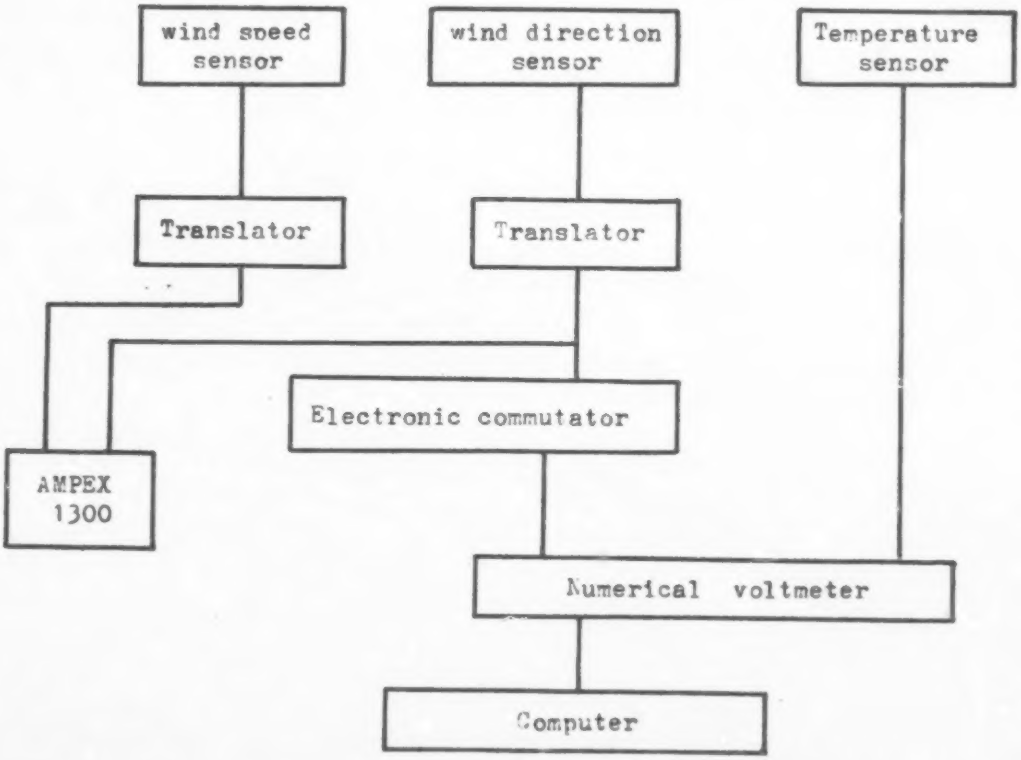
The data acquisition system consisted in a real time treatment using computer (HEWLETT - PACKARD, type 21 - 16 B). Table 2 shows the block diagram of treatment.

.../...

TABLE 1 : SELECTED INSTRUMENTS

ELEMENT	SENSOR	LEVEL
wind wind fluctuations	3 U V W Gill anemometers	12.2 - 20.2 m 31.6 m
	2 cup anemometers	12.2 m - 31.6 m
	1 Bivane 1 Profeller vane	7.4 m
Temperature	quarty thermometer	11.6 m - 31 m

TABLE 2 : BLOCK DIAGRAM OF TREATMENT


wind speed sensor
wind direction sensor
Temperature sensor
Translator
Translator
Electronic commutator
AMPEX 1300
Numerical voltmeter
Computer

Then, climatological records of temperature, wind speed, azimuth and elevation angles, and standard deviation of each quantity were available during different periods of sampling time (10 mn, growing to 3 h) over different averaging times (from 5 s to 10 mn).

The analysis of these meteorological quantities allowed the study of the variation of the intensities of turbulence with stability, wind speed and height above the surface. Then, we deduce a decrease law of $\frac{\sigma_u}{U}$, σ_θ -longitudinal and lateral intensities of turbulence- with increasing atmospheric stability, wind speed and height (fig. 7). The effect of these was somewhat different on the vertical intensity of turbulence $-\sigma_\varphi-$.

Using the HAY - PASQUILL method of moving averages, we obtained the influence of the averaging and sampling times on the intensities of turbulence. Then, derived from TAYLOR's theory, the rate of dispersion of particles emitted from a fixed point source is written :

$$\overline{y^2} = \overline{v^2}_{(t/\beta\,,T)}\; t^2 \qquad \text{lateral direction,}$$

$$\overline{z^2} = \overline{w^2}_{(t/\beta\,,T)}\; t^2 \qquad \text{vertical direction.}$$

- t is the diffusion or travel time,
- $\overline{v^2}_{(t/\beta,\,T)}$ and $\overline{w^2}_{(t/\beta\,,T)}$ are the mean square value of the moving average velocity process formed with averaging time t/β during the sampling time T.

$$\overline{v^2}_{(t/\beta\,,T)} = \overline{v^2}\int_0^\infty F_{Eul}(n)\,\frac{\sin^2(n\,\pi\,t/\beta)}{(n\pi\,t/\beta)^2}\left[1-\frac{\sin^2 n\pi T}{(n\pi T)^2}\right]dn$$

- $F_{Eul}(n)$ is the Eulerian spectrum.
- β is the Lagrangian to Eulerian time scale ratio (ranging from 2 in very unstable to 6 in stable). .../...

This may be written in an indentical form when we replace the diffusion time t by the down-wind distance x ($x = U\,t$, U is the mean velocity) and the mean square values of velocity fluctuations $\overline{v^2}$ and $\overline{w^2}$ by the intensities of turbulence Iy and Iz .

$$\left(Iy^2 = \frac{\overline{v^2}}{U^2} \ , \quad Iz^2 = \frac{\overline{w^2}}{U^2} \right)$$

$$\sigma y = \sqrt{\overline{y^2}} = Iy \ (t/\beta \, ,T) \ x$$

$$\sigma z = \sqrt{\overline{z^2}} = Iz \ (t/\beta \, ,T) \ x$$

Using the standard deviation of azimuth and elevation wind-direction angle ($\theta \sim \frac{v}{U}$, $\varphi = \frac{w}{U}$) , this may be written :

$$\sigma y = \sigma_\theta \ (t/\beta \, ,T) \ x$$

$$\sigma z = \sigma_\theta \ (t/\beta \, ,T) \ x$$

Then, we can adapt the PASQUILL's dispersion parameters to the turbulent characteristics of the site. For instance, in the case of strong winds associated to a neutral stability (including the MISTRAL), we present in Fig. 8 and Fig. 9 the influence of the averaging and sampling times on σ_θ and the corrected rate of lateral dispersion (with 10 mn sampling) compared to PASQUILL's categories C and D. In Fig. 10 and Fig. 11 we present separately the influence of wind speed and surface routhness related to the value of $\sigma_\theta U$ which appears as a good concept to characterize σy .

Assuming that the flow remains approximately stationnary over periods of one, two or three hours, we studied the influence of the sampling time on the rate of dispersion in order to correct the ratio of 3 hours to 10 mn concentrations.

.../...

Using the empirical form :

$$\sigma_\theta(T_i) = \left(\frac{T_i}{T_o}\right)^p \quad \sigma_\theta(T_o)$$

$$\sigma_\varphi(T_i) = \left(\frac{T_i}{T_o}\right)^q \quad \sigma_\varphi(T_o)$$

Then, we deduced the variations of the exponents p and q with stability, wind speed and height above the surface. We present in Fig. 12 the results obtaines for p. It is important to note that σ_φ shows very little increase with sampling time and it was difficult to dissociate the variability of mean flow from the turbulent regime.

Assuming a Gaussian distribution for the concentrations, the relationship between the maximum ground level concentration and the sampling time is given by the following formula :

$$\chi_{max} \sim \frac{Q}{\pi \ \sigma_{y_T} \sigma_{z_T}} \exp\left\{-\frac{y^2}{2\sigma^2_{y_T}}\right\} \exp\left\{-\frac{H^2}{2\,\sigma^2_{z_T}}\right\}$$

where Q is the source strength and H is the effective stack height.

Then, we deduced the effect of sampling time on concentrations using the empirical form mentionned earlier.

$$\chi_{max}(T_i) = \left(\frac{T_i}{T_o}\right)^{-M} \chi_{max}(T_o)$$

Fig. 13 shows the results obtained for $\frac{\chi_{max}\,(3\ h)}{\chi_{max}\,(10\ mn)}$ at 12.2 m and 31.6 m levels for different wind velocities and atmospheric stabilities. It is important to note that this ratio decrease with decreasing wind speed (maximum value for strong winds ≃ 0.75) , it

.../...

shows in neutral stability the higher values and shows very little variation with height.

IV - CONCLUSION

In this paper we tried, essentially, to present a method which takes into account as much as possible the characteristics of a given site. The study is not yet completed, and particularly the part concerning the thermal structure and its correlation with other meteorological parameters. We hope to be able to give you more results in the next meeting.

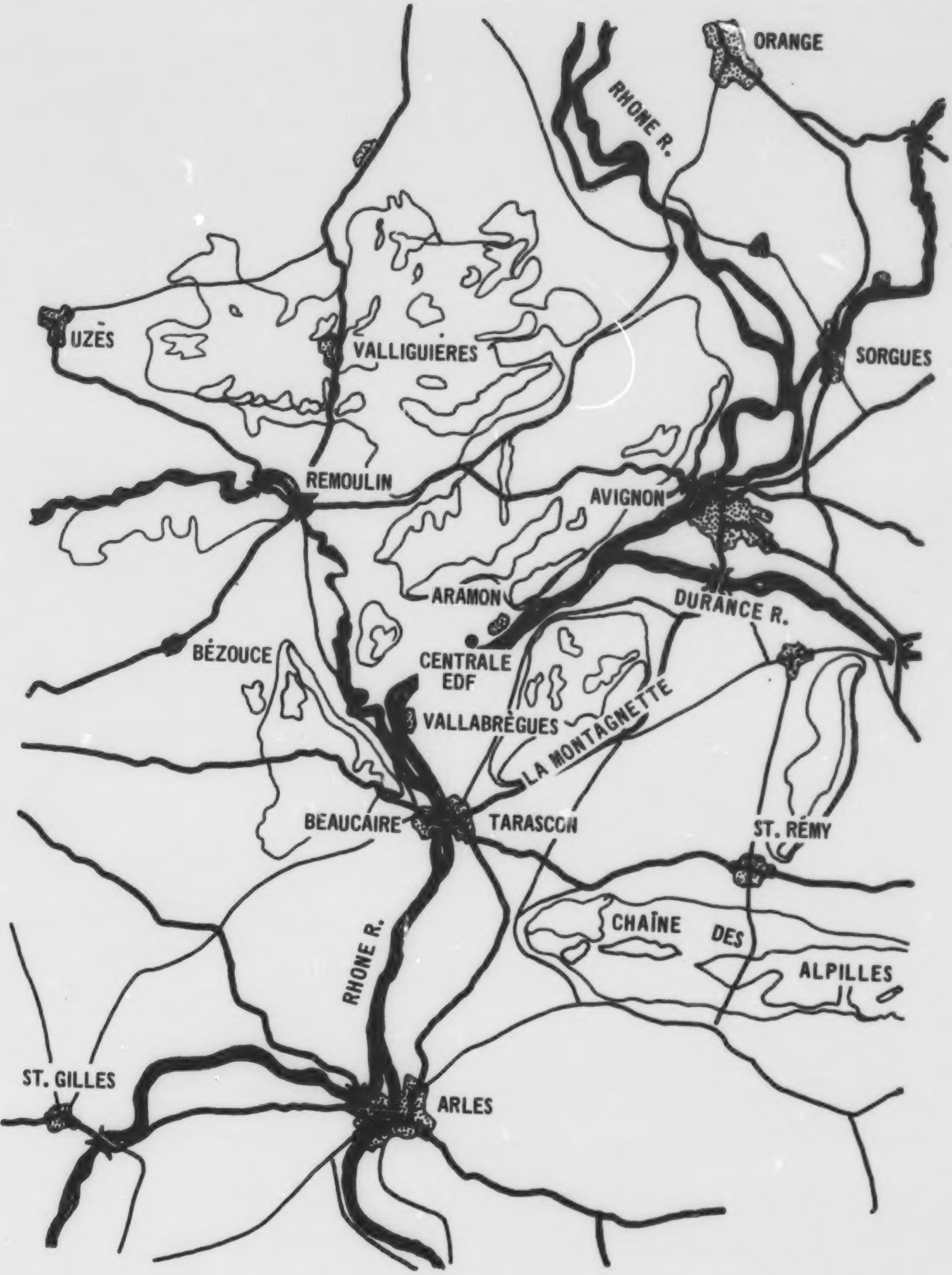

ORANGE
RHONE R.
UZÈS
VALLIGUIÈRES
SORGUES
REMOULIN
AVIGNON
ARAMON
DURANCE R.
BÉZOUCE
CENTRALE
EDF
VALLABRÈGUES
LA MONTAGNETTE
BEAUCAIRE
TARASCON
ST. RÉMY
CHAÎNE
DES
ALPILLES
RHONE R.
ST. GILLES
ARLES

Fig: 1

DİRECTİON	OCCURRENCE	DİRECTİON	OCCURRENCE
20	46	200	36
40	13	220	34
60	3	240	12
80	5	260	14
100	8	280	21
120	14	300	28
140	20	320	56
160	28	340	147
180	43	360	244
CALM WİND 228			

Fig:2 - SUMMARY OF WİND DİRECTİON OCCURRENCE - per 1000 - AT ORANGE - CARİTAT (YEAR 1953 - 1962)

MISSING

Fig: 3

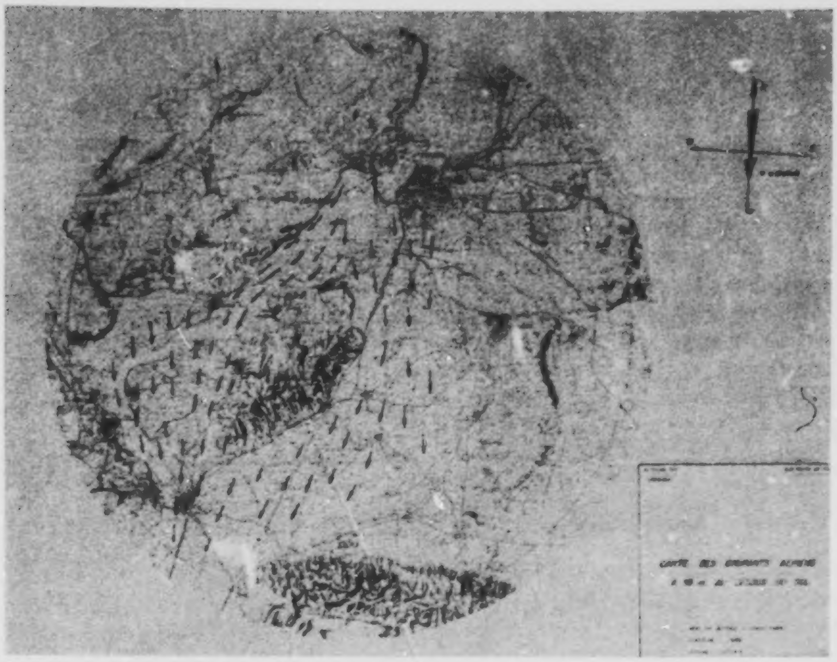

CARTE DES COURANTS AERIENS

Fig: 4a

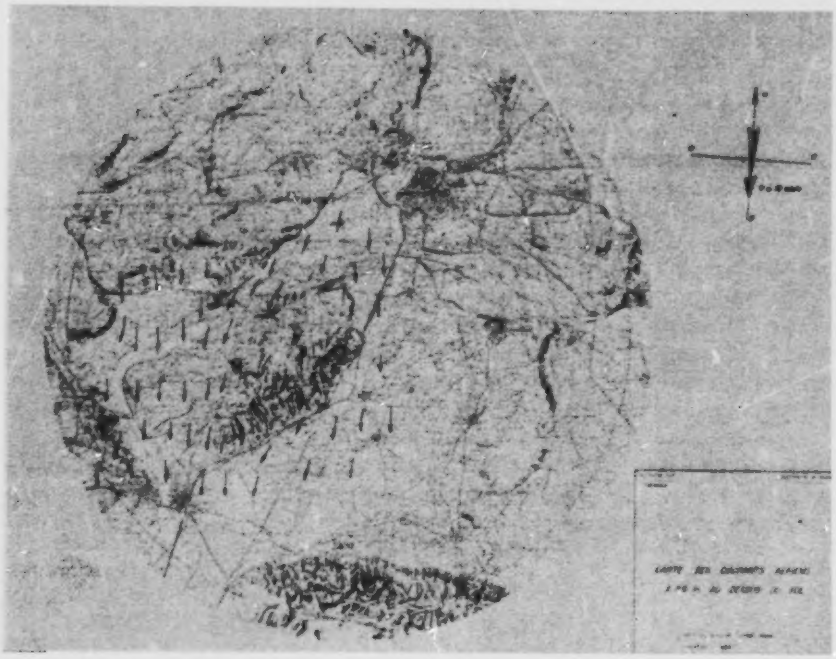

CARTE DES COURANTS AERIENS

Fig: 4b

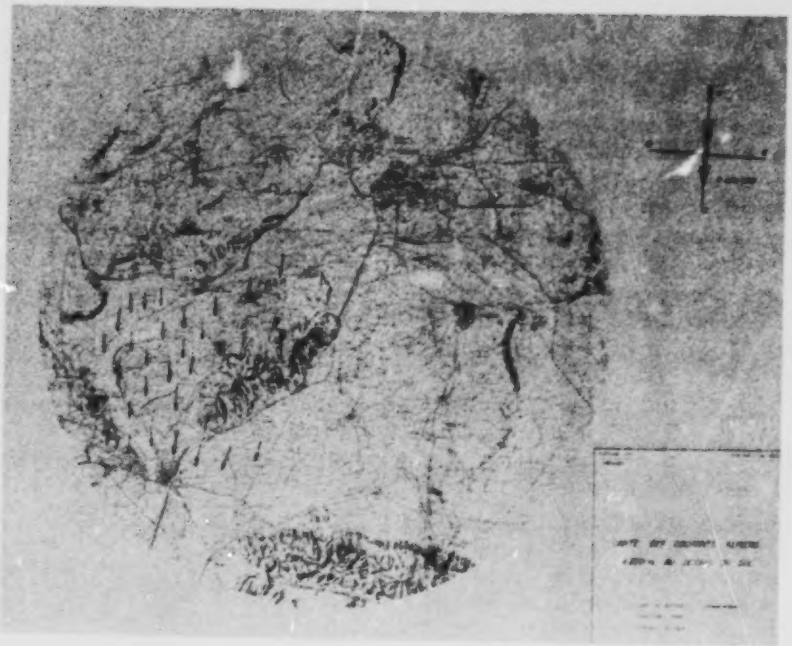


Fig: 4c

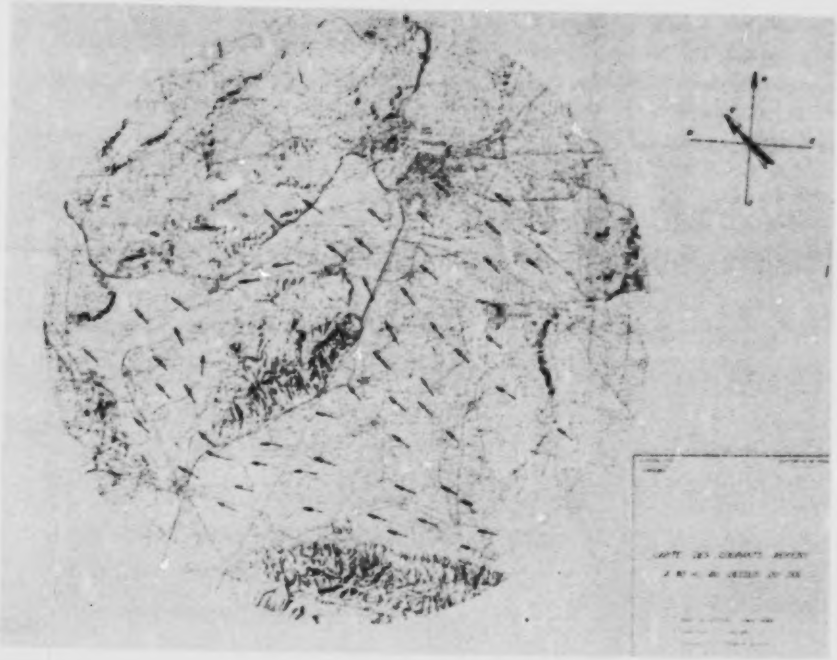


Fig: 5a

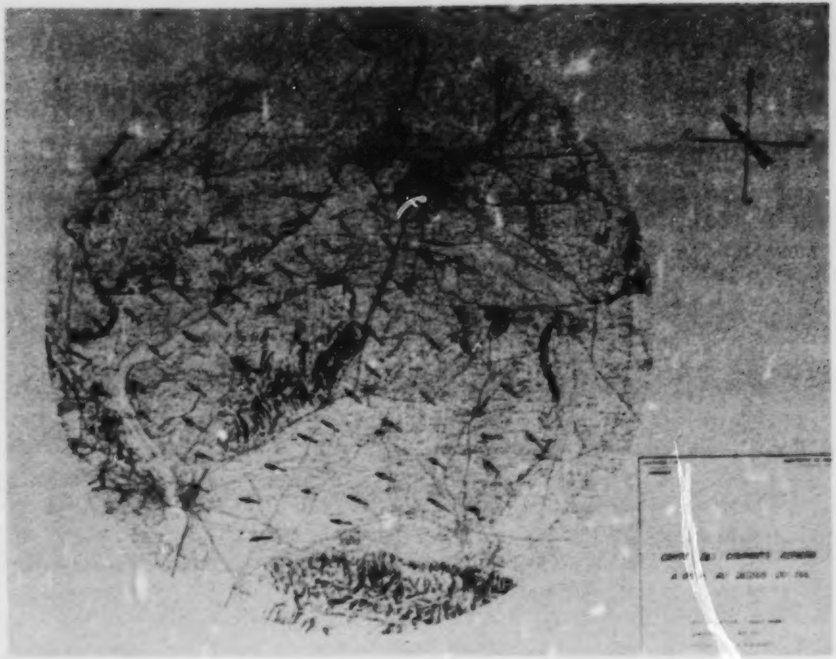


Fig: 5b

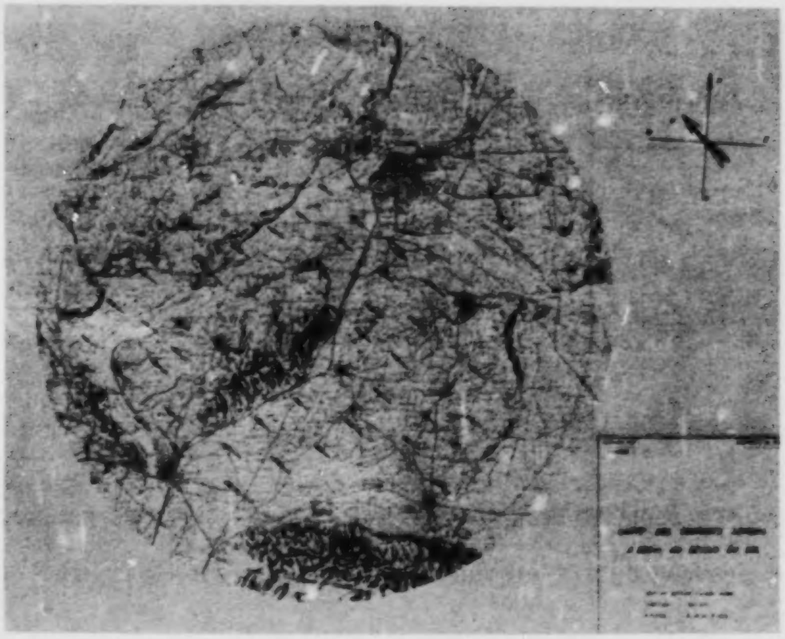


Fig: 5c

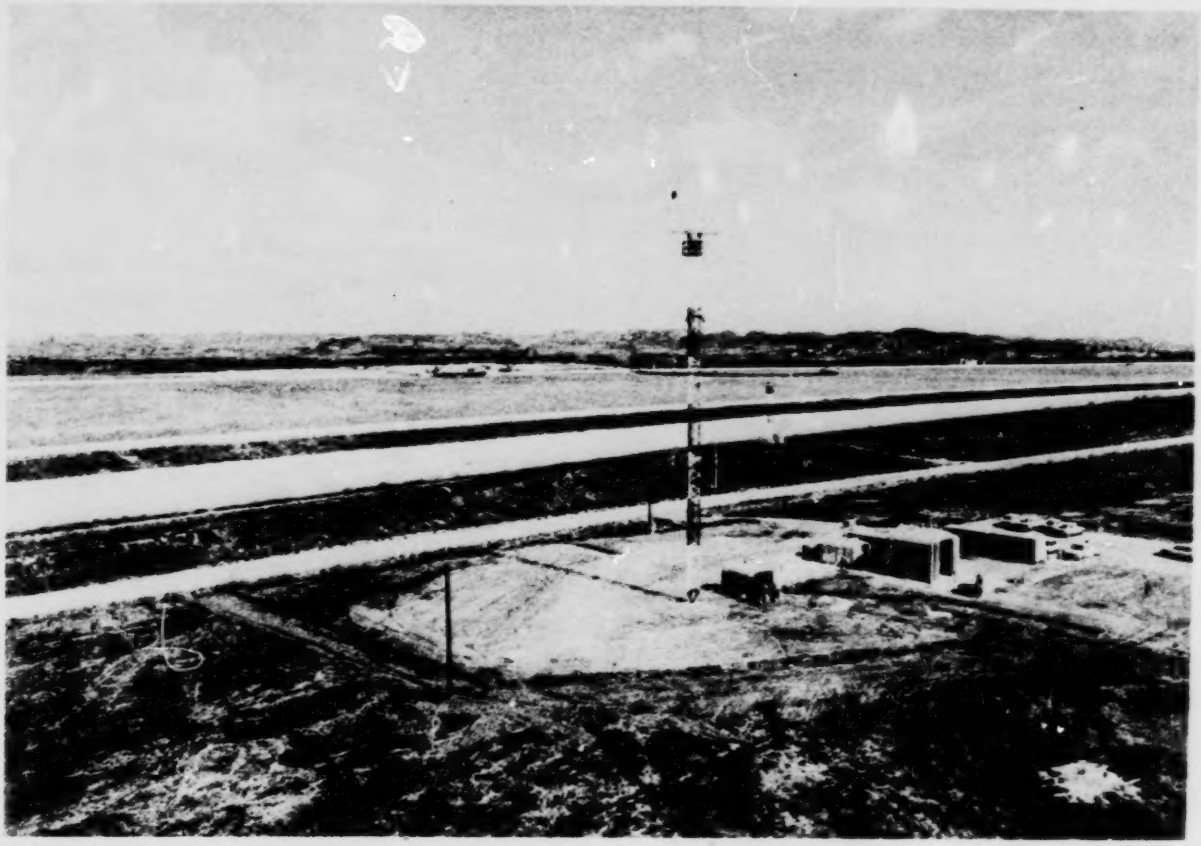


Fig: 6

LEVELS	7.4 m	12.2m	20.2m	31.8m
UNSTABLE $\Delta T < -.5°C$				
U > 8m/s		0.21	0.20	0.18
4 < U < 8		0.23	0.21	0.20
2 < U < 4		0.28	0.24	0.24
U < 2		0.36	0.33	0.33
NEUTRAL $-.5 < \Delta T < .5°C$				
U > 8m/s		0.17	0.17	0.15
4 < U < 8		0.21	0.20	0.18
2 < U < 4		0.24	0.21	0.20
U < 2		0.27	0.34	0.22
STABLE $\Delta T > .5°C$				
U > 8m/s		0.16	0.14	0.13
4 < U < 8		0.18	0.18	0.15
2 < U < 4		0.18	0.15	0.15
U < 2		0.19	0.17	0.14

$\frac{\sigma_U}{U}$ FOR AN AVERAGING TIME OF 5s AND A SAMPLING TIME OF 10mn

LEVELS	7.4 m	12.2 m	20.2m	31.8m
UNSTABLE $\Delta T < -.5°C$				
U > 8m/s	11.8	10.4	8.8	9.1
4 < U < 8	13.3	11.8	11.3	10.7
2 < U < 4	14.7	14.0	12.8	12.3
U < 2	19.5	17.3	15.3	13.3
NEUTRAL $-.5°C < \Delta T < .5°C$				
U > 8m/s	9.5	8.3	8.1	7.8
4 < U < 8	10.8	9.6	8.8	8.6
2 < U < 4	12.2	11.4	10.4	9.0
U < 2	12.7	11.8	11.5	10.8
STABLE $\Delta T > .5°C$				
U > 8m/s	8.3	6.8	6.1	5.7
4 < U < 8	8.9	6.9	5.8	4.4
2 < U < 4	10.2	6.9	6.0	4.7
U < 2	10.8	7.0	5.9	5.3

σ_θ (in degrees) For an averaging time of 5s. and a sampling time of 10mn.

LEVELS	7.4 m	12.2m	20.2m	31.8m
UNSTABLE $\Delta T < -.5°C$				
U > 8m/s		3.5	4.1	4.4
4 < U < 8		4.2	4.9	5.3
2 < U < 4		6.1	6.6	7.3
U < 2				
NEUTRAL $-.5°C < \Delta T < .5°C$				
U > 8m/s		2.8	3.9	4.4
4 < U < 8		3.1	3.7	4.1
2 < U < 4		1.7	2.0	2.2
U < 2				
UTABLE $\Delta T > .5°C$				
U > 8m/s		2.7	2.9	3.1
4 < U < 8		1.7	1.9	2.0
2 < U < 4		1.2	1.4	1.5
U < 2				

σ_φ (in degrees) For an averaging time of 5s and a sampling time of 10mn

Fig: 7

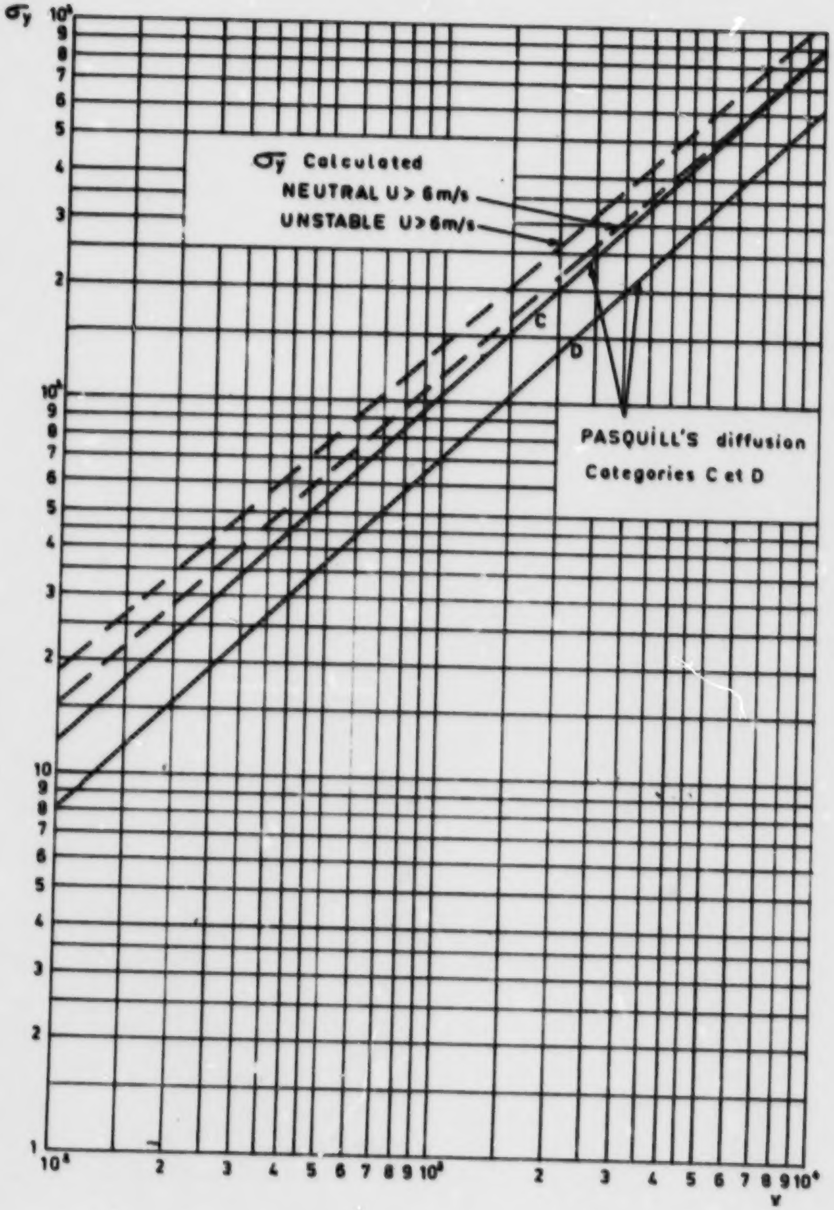

σ_y
10^3
10^2
10
1
$\sigma_{\bar{y}}$ Calculated
NEUTRAL U > 6m/s
UNSTABLE U > 6m/s
C
D
PASQUILL'S diffusion
Categories C et D
10^2
10^3
10^4
y

Fig: 9

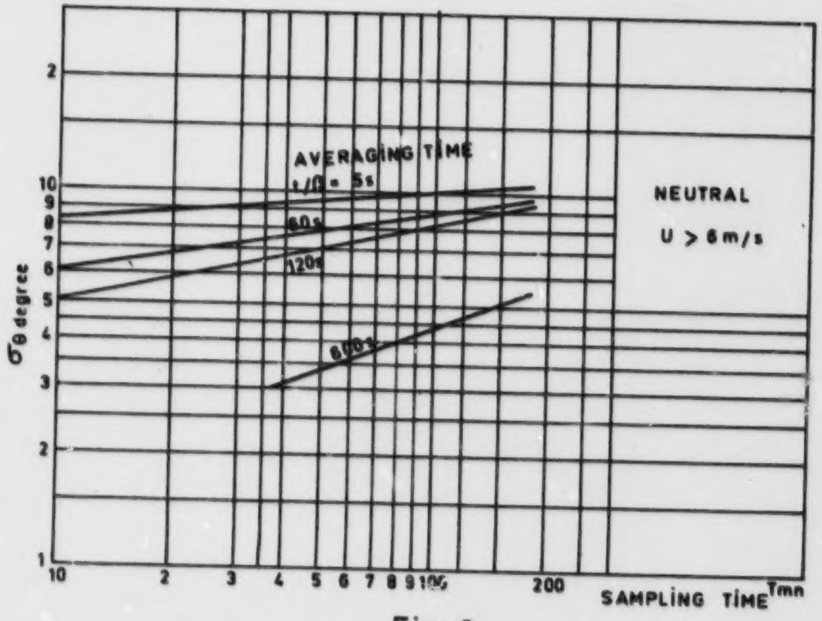

σ_θ degree
AVERAGING TIME
t/Δ = 5s
60s
120s
600s
NEUTRAL
U > 6 m/s
10
10^2
200
SAMPLING TIME Tmn

Fig: 8

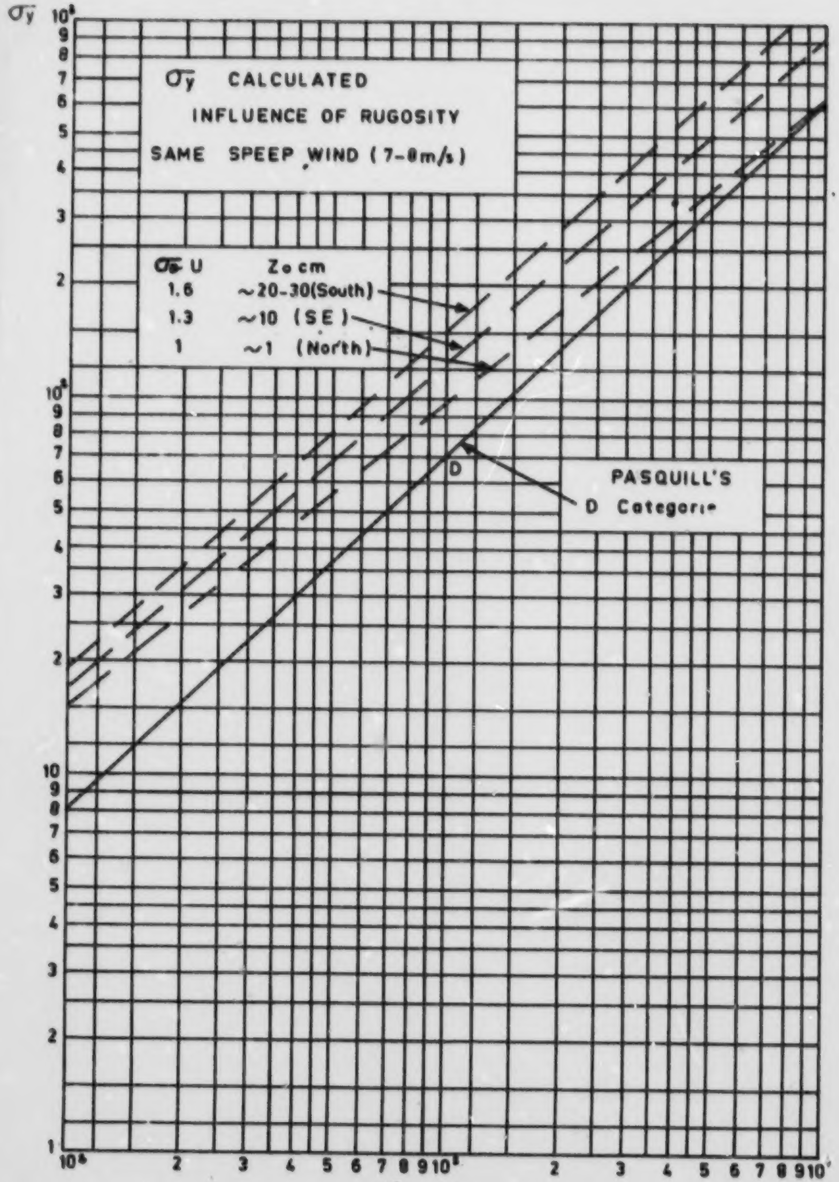

σy
σy CALCULATED
INFLUENCE OF RUGOSITY
SAME SPEEP WIND (7-8m/s)
σθ U Zo cm
1.6 ~20-30(South)
1.3 ~10 (SE)
1 ~1 (North)
PASQUILL'S
D Categorie
D
10³
10²
10
1
10¹
10²
10³
x

Fig: 11

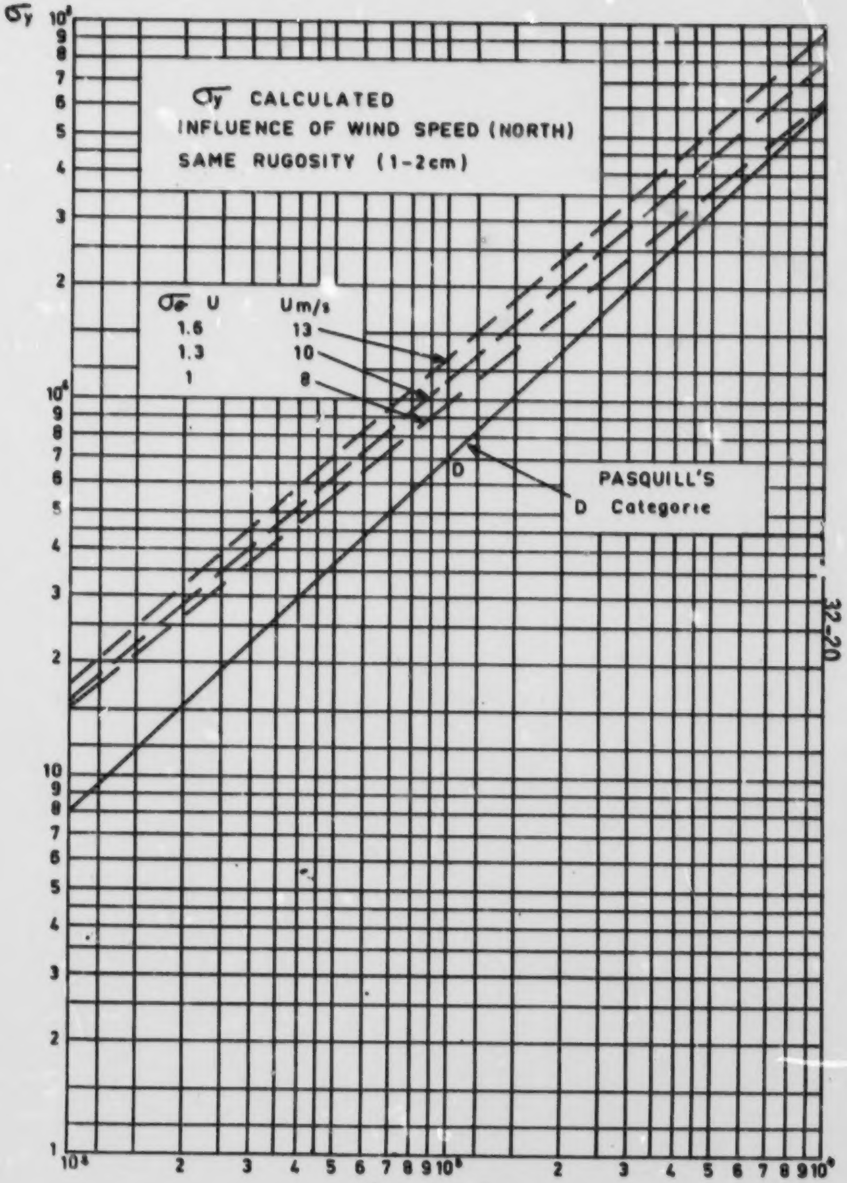

σy
σy CALCULATED
INFLUENCE OF WIND SPEED (NORTH)
SAME RUGOSITY (1-2cm)
σθ U Um/s
1.6 13
1.3 10
1 8
PASQUILL'S
D Categorie
D
10³
10²
10
1
10¹
10²
10³
x

Fig: 10

LEVELS	7.4 m	12.2 m	20.2 m	31.6 m
UNSTABLE $\Delta T < -.5^{\circ}C$				
$U > 6 m/s$	0.13	0.13	0.14	0.155
$4 < U < 6$	0.18	0.21	0.22	0.225
$2 < U < 4$	0.22	0.24	0.27	0.29
$U < 2$		0.37	0.41	0.46
NEUTRAL $-.5^{\circ} < \Delta T < .5^{\circ}C$				
$U > 6 m/s$		0.08	0.08	0.08
$4 < U < 6$	0.14	0.135	0.13	0.13
$2 < U < 4$		0.23	0.22	0.22
$U < 2$		0.35	0.34	0.30
STABLE $\Delta T > .5^{\circ}C$				
$U > 6 m/s$		0.07	0.07	0.06
$4 < U < 6$	0.33	0.36	0.365	0.375
$2 < U < 4$	0.34	0.34	0.39	0.43
$U < 2$		0.37	0.375	0.39

Fig: 12 - p Values: $\frac{\sigma_\theta\,(3h)}{\sigma_\theta\,(10mn)} = \left(\frac{3h}{10mn}\right)^{p}$

LEVELS	7.4 m	12.2 m	20.2 m	31.6 m
UNSTABLE $\Delta T < -.5^{\circ}C$				
$U > 6 m/s$		0.63		0.58
$4 < U < 6$		0.51		0.49
$2 < U < 4$		0.44		0.375
$U < 2$		0.26		0.20
NEUTRAL $-.5^{\circ} < \Delta T < .5^{\circ}C$				
$U > 6 m/s$		0.75		0.75
$4 < U < 6$		0.62		0.60
$2 < U < 4$		0.485		0.50
$U < 2$		0.285		0.31
STABLE $\Delta T > .5^{\circ}C$				
$U > 6 m/s$		0.79		0.81
$4 < U < 6$		0.33		0.31
$2 < U < 4$		0.30		0.22
$U < 2$		0.25		0.20

Fig: 13 - $K = \frac{\chi\,(3h)}{\chi\,(10mn)}$ Concentration - ratio 3h - 10mn

Chapter 33

RESEARCH PROGRAM OF MODEL DEVELOPMENT BRANCH OF THE E. P. A.

by

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Meteorology Laboratory
U. S. Environmental Protection Agency

5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

Air Quality Model Development Program

by

Douglas G. Fox, NOAA

A concise review of the existing and anticipated research and development activities of the Model Development Branch, Meteorology Laboratory, EPA is presented. Long term goals are outlined as are interim steps in the achievement of these goals. In particular, five areas of activity are considered, urban meteorology, atmospheric structure modeling, atmospheric transformation modeling, model validation and simplification, and physical modeling.

In the interests of time and the fact that Dr. Fox has not been readily available for discussions, this paper is now included without any editorial review or corrections.

I. Introduction

The research performed within our branch of the Meteorology Laboratory is determined on an annual basis by the EPA-Office of Research and Development (EPA/ORD) Program Planning System. This system formalizes needs of the so called "user" community, evolves research objectives, manages ROAPS (Research Objective Achievement Plans) and disseminates the finished products. While the ROAPS change from year to year there is, hopefully, sufficient stability within this system to identify general areas of research based essentially on ROAP history, current EPA policy and problems and availability of personnel.

The research in our branch is very much multidisciplinary consisting of experimental, theoretical and air pollution meteorologists, an applied mathematician, an aerospace engineer and a physical chemist as well as technicians and other support personnel. At present we are organized into five areas of research; urban meteorology, atmospheric structure calculations, atmospheric transformation modeling, diffusion model validation and simplification, and physical modeling. In the following sections each of these areas will be discussed in some detail.

II. Urban Meteorology

A major use of air quality simulation models is in developing and evaluating implementation plans to meet air quality standards in highly polluted urban areas. A number of considerations limit the validity of currently used models (AQDM, CDM). The comprehensive Regional Air Pollution Study (RAPS) has evolved as an attempt to improve urban, indeed regional, air quality modeling. The major emphasis within this area of our research is on supporting the RAPS with experimental measurements as well as development of the RAPS model.

Two types of air quality simulation models are currently used in urban areas, namely the multiple source Gaussian diffusion model (1) which in practice uses a single wind velocity, stability and mixing depth and more complex mass balance models requiring a field of wind magnitude and direction and boundary layer structure. (2-4) Obviously each model class is appropriate for different problems. The complex models are required to calculate short term concentrations of reactive pollutants and to calculate concentrations during episodal conditions. The MSUDM's are seemingly capable of relating ambient air quality to source emissions on a climatological basis and on a short time basis during strong and persistent meteorological conditions.

The meteorological portion of the complex models is obviously of significance. In order to make such models more generally useful, efficient means of calculating urban wind fields must be developed. Since very little is known in general about the boundary layer within a city, a first task is to accumulate data of sufficient extent and quality to enable a preliminary understanding of urban meteorology. To this end we have performed a number of studies of the atmospheric structure over urban areas. The details of the urban-rural temperature contrast, the distribution of temperature in a city, the distribution of air quality in a city and the dispersion characteristics of urban areas have all been subjects of previous studies.

Current activities are focussed on a continued determination of the atmospheric structure, particularly during times of transition such as dawn and dusk, on measurement of the fine scale variability expected in air quality and meteorological parameters within the urban area, and on the determination of components of the energy balance at the urban surface.

Experiments were performed last summer (1973), in February 1974 and are currently underway aimed at a clearer understanding of the boundary layer structure differences between the urban area and rural background during sunrise and sunset. The experiments consist of making measurements on the surface with an instrumented van and a mobile lidar system. These operate from outside the city into the city providing essentially single lines of surface temperature and mixing depth (assuming the lidar return which is related to the aerosol content delineates the mixing depth). As well an instrumented helicopter is used to make measurements of the atmospheric structure, i.e., temperature, pollutant concentration and humidity, over the city. A rather typical indication of the urban influence on the local meteorology is shown in Figure 1. (5,6) Often however the general pattern is not obvious and a great deal more data are required to quantify any results. The boundary layer structure in the form of a depth of the mixed layer is a direct input to the Gaussian diffusion model. For the more complex models, studies of the boundary layer structure will be able to provide quantitative data. From such data it should be possible to establish simple models of urban meteorological influences given conventional measurements such as an airport sounding.

An essential element in any understanding of urban meteorology is determination of the spatial distribution and temporal variation of the energy balance at the urban surface. Urban areas affect the airflow mechanically by acting as obstacles to the wind and thermally by either absorbing or emitting heat and water vapor differently from their surroundings. These differences give rise to the well documented urban heat island circulation as well as a number of other related phenomena. Any attempt to quantify temporal changes in urban structure cannot proceed without a comprehensive set of measurements of the local energy balance. Measurements will be made to determine the flux of heat and moisture at various heights above the city surface by using a tethered balloon.

These will be coupled with airborne radiation measurements of both long wave and solar radiation at various heights throughout the mixed layer so that radiative flux divergences associated with the urban area can be calculated. These measurements will assist in determination of the relative significance of aloft and surface heating on urban meteorology as well as the more general consideration of the relative importance of mechanical and thermal forcing on the urban boundary layer structure.

Finally a major concern of air quality simulation models is the mixing environment of the city, namely the magnitude of dispersion coefficients as a function of meteorological conditions and, say, urban land use. An early attempt to determine the mixing character of a city was done by Pooler as reported in McElroy and Pooler. (7) A much wider scope of conditions however must be studied in order to truly define the dispersion environment of a city. A primary concern here is the manner in which point, line and complex sources become integrated into the general air quality of a region. In order to provide information in this area we will study dispersion close to such sources. In associated work long path monitors (tunable diode laser instruments) are under development by the Chemistry and Physics Laboratory for the purpose of measuring average pollution along a path.

The important question posed within an urban area is -- how does a point measurement of pollution relate to the general background of that pollutant. A series of experiments are being designed to answer this and associated questions. Some information has already been accumulated. The Stanford Research Institute in an attempt to validate their urban mobile source CO model performed experiments in St. Louis and San Jose.(8) Their experiments confirmed that under strong winds a standing eddy could exist within typical street canyons. The concentration gradient of CO from bottom to top of the canyon depends upon such factors as the wind magnitude and direction, but generally is not greater than a factor of two. Much larger variations probably occur as one extends the area over which the average is calculated to something in the order of 1 km square.

The variability of pollutant concentration over a one kilometer area could be very great depending upon the pollutant and for example upon being inside or outside a plume from a specific source. In order to obtain a baseline measurement of variability one might consider wind magnitude and direction, the temperature structure and the turbulence structure variation over the area. Since these characterize the dispersion climate of the area one would expect that any pollutants with no sources within the area (i.e., background pollutants) would trace the air motion and have a variability associated with the variability of the air motion. Thus such measurements might be expected to determine a baseline area variability and hence an indication of the significance of such variation for grid-type air quality simulation models. Related experiments are needed to characterize secondary pollutant behavior near the primary pollutant sources. Such work requires cooperative efforts between chemists and meteorologists.

III. Atmospheric Structure Calculations

Different levels of meteorological information are required by the two types of air quality models generally utilized. The flow field requirements of most common Gaussian diffusion models are a local wind vector, a mixing depth, and an atmospheric stability. It is felt that significant improvement of such models could result if more meaningful mixing information were provided particularly for an urban area.

For the urban problem, results of the work in our urban meteorology program will be applied to establish improved mechanisms for calculating mixing depth and for incorporating this mixing depth into the diffusion models. The atmospheric structure model required here might be one which would relate the depth of the mixing layer over a city to the routinely available rural sounding. It could allow for such things as wind turning with height (as a function of stability) and temporal and spatial urban texture dependent mixing depth calculations. An example for the Gaussian founded AQDM type model, might be to add some horizontal spatial variability in the meteorological boundary conditions. The development of such an AQDM is currently underway. The air quality diffusion portions of such a model are quite straightforward. In the conventional AQDM Gaussian dispersion formulas are applied to each point and area source and all the contributions are summed at particular receptors. One wind velocity and one mixing depth characterize the urban flow. Development of improved models utilizing a more comprehensive flow field are underway. But the major difficulty with such an advance is how to calculate the flow field. The RAPS will provide a substantial data base from which to study urban flow fields. Twenty-five surface stations, half with 30 meter towers and the other half with 10 meter towers, will provide a vast array of wind measurements. These coupled with a regular set of radiosondes and "pibal" ascents will allow development of objective analysis techniques appropriate for urban meteorology.

The current approach to urban objective analysis is through data interpolation and smoothing schemes. Existing models which require wind fields obtain them from surface measurements by polynomial interpolation. For example, to calculate $A(x,y)$ given a measurement $\hat{A}(\hat{x},\hat{y})$ one could use

$$A(x,y) = \sum_i W_i(r)\,\hat{A}(\hat{x},\hat{y}) \Big/ \sum_i W_i(r)$$

where $r = \sqrt{(x-\hat{x}_i)^2 + (y-\hat{y}_i)^2}$ and $W_i(r)$ is the interpolating function generally given by something like

$$W_i(r) = \frac{R^2 - r^2}{R^2 + r^2} \qquad r \leq R$$

$$= 0 \qquad r > R$$

and R = radius of a circle about (x,y) and is considered to be the radius of influence of the measurement.(9) Obviously the size of R determines the smoothness of the wind field. A number of improvements of this technique by using for example fourier weighting can be made and are being investigated currently. An associated problem is the specification of the third dimension of the flow field. Currently the third dimension can be estimated by maintaining the surface pattern and decreasing the magnitude of the velocity with height according to the indications of local soundings. Actual measurements however indicate a much more complex structure aloft. We are currently establishing a program to synthesize and improve objective analysis schemes for urban areas. Initially this work is being done via extramural funding. In developing such a program we will strive toward an analysis scheme which produces meaningful urban flow fields using minimal input data. After experience with the RAMS data objective techniques should progress from simply data assimilation to take on a more diagnostic note. Dynamically meaningful constraints such as nondivergence (or divergence), conservation of momentum, etc., can be introduced into the analysis by utilizing the techniques of variational calculus. An orderly progression from analysis to prognosis is envisioned.

Work began last year on a rather comprehensive prognostic model for the air flow in an urban area. Our so called Wind And Temperature Prediction Code (WATPC) is a solution of three dimensional equations of motion along with the temperature equation for an urban region. The model predicts the flow field over 1km by 1km horizontal grid points with a total area of approximately 40 by 40km. Current aspects of the development include bottom and lateral time dependent boundary conditions, turbulent transport parameterizations and pollutant diffusion submodels. WATPC will be most useful for predicting flows during episodal conditions when local thermal and mechanical inhomogenietes have a determining influence on the flow field structure. In order to do this we (10) have developed a surface energy budget model which is capable of calculating the heat flux boundary condition at the lowest grid level. A parameterization of the surface mechanical roughness is yet to be included in the lower boundary condition.

In any meteorological model of less than hemispheric scale one must consider the lateral boundary conditions. They must allow the correct propogation of large scale flow features into the smaller scale model as well as allowing the smaller scales to properly influence the larger scales. In general such requirements can be specified by nesting a fine grid model within a larger grid. In the urban case the larger grid model would be on the mesoscale with a grid spacing of roughly 20km square which itself will be nested within a larger scale meteorological model with grid spacing on the order of 200km. The details of specifying boundary conditions properly is a problem of current research which does not have a generally accepted formal solution. Nevertheless, a few models are currently in existence (11-12) which could be useful for providing the lateral forcing. Developments in this area while not actively pursued by our branch are closely monitored. In fact the mesoscale modeling of Anthes (12) is funded by a grant from the Meteorology Laboratory.

In order to perform modeling to predict urban meteorological structure it is first necessary to determine the equations which describe the meteorological structure. The conventional equations of dynamic meteorology are derived from the Navier-Stokes equations for a compressible, stratified, rotating fluid. For the temporal and spatial scales of interest we can eliminate such things as compressibility, however most of the other conventional approximations of meteorology are not necessarily appropriate. In particular, it is not clear that assuming the urban atmosphere is in hydrostatic equilibrium is justified nor is it reasonable to restrict the dimensionality to less than three. Although there is no good data available one might envision an idealization of the spectrum of energy in an urban area to be rather flat with a tendency to increase for scales smaller than 2km until about .1km where it might decrease. The point to convey is the rather complex nature of the spectrum as opposed to say larger scale meteorological modeling,the flow does not exhibit a simple decay. The use of an eddy viscosity in the equations for modeling such conditions is not sufficient. Rather it is necessary to delve more into the theory of second order turbulence closure. The function of such theory is to stimulate the [illegible] nature of subgrid actions (i.e., account for transfers occurring at scales smaller than the scale on which the equations are solved). (13) The subgrid resolution problem is a recurring one which we will discuss in other contexts subsequently. In order to determine the proper closure mechanisms, we are funding an extramural research effort. Such effort includes work on the general nature of second order closure by a group at Pennsylvania State University headed by Professor John Lumley; (14) work related to some specific mechanisms and the testing of same by ARAP under Dr. Colman Donaldson; (15) and a small effort to attempt the validation of such mechanisms by Dr. Steven Orszag at Flow Research, Inc. (16)

At the present time WATPC uses a constant eddy viscosity. We plan on a progressively improving treatment with, as the first improvement, a ratio of K_H/K_V different from unity. The final model would, we now envision, treat turbulence by using a closure based upon the turbulent dissipation and the turbulent kinetic energy. Thus we would add transport equations for these two quantities and introduce an eddy viscosity which is a function of ϵ and e. Figure 2 shows some preliminary results from WATPC.

While this fundamental and yet very necessary research is progressing, it is useful to develop methods which will provide answers as quickly as possible. Such models are needed for the urban area but may find even greater use outside of urban regions. Often, the regions in which we are asked for a wind field are ~~ones~~ where for one reason or another the measuring station is not representative of the meteorology. Such situations generally have some strong local forcing such as a diurnally varying land-sea temperature difference, or strong topographical influences. Situations of this type lend themselves to modeling using some of the aforementioned simplifying assumptions. In particular, we have a program for modeling dispersion in complex terrain. In a similar vein we have done some work on modeling the sea breeze and other temperature differential type phenomena. Some examples are the work of Professor Lyons at the University of Wisconsin, Milwaukee who is modeling the dynamics of an urban lake breeze, (17) and recently completed research by Professor Moroz at Pennsylvania State University on a similar problem. (18)

Consider the problems of modeling in complex terrain. Given, for example, a smelter in the western U. S. located in terrain with very complex features and as much as 1,000m elevation differences, the question is asked - How often, and for how long will the plume from the smelter impact on the mountain slope? In order to deal with the problem of dispersion in such terrain it is necessary to have a reasonable model of the flow field. In order to model such flows one could undertake an effort very similar to our WATPC. However, a model is required now not in five years. A quick model can be done if one applies simplifications of the equations of motion. For example, one could consider, in descending order of complexity, models based upon (1) multilevel integrated equations, (2) potential flow and (3) temperature-pressure forcing.

Multilevel modeling uses the well established approximation of treating the atmosphere as consisting of layers each of which are reasonably uniform but which exert an effect upon one another. Perhaps the most well known of this type model is the one developed by Lavoie (19) for mesoscale lake effect storms. In the field of pollution, Dr. Tingle of H. E. Kramer, Inc. has developed a model of this type for calculating the flow over complex terrain. (20)

Potential flow models have been used in fluid mechanics for many varied applications. They consist of a numerical solution of some form of an elliptic equation. A property of such equations is to distribute a function applied at the boundaries throughout the domain. Thus such equations are capable of representing the flow only to the extent that it is forced by the surface. They are very handy in representing the flow over major topographic features. Dr. Lenz of Intercomp, (21) has developed such a model which is currently being evaluated by EPA. The disadvantage of such a flow model is its inability to represent stagnation and generally stable conditions. Various artificial mechanisms have been suggested to overcome such difficulties, however, none have been sufficiently well verified for general use.

Finally Dr. Fosberg, U. S. Forest Service and colleagues at Colorado State University have developed a fascinating, simple, yet useful model. (22) The desired object was to develop an analytical relationship between surface temperature and wind field, since surface temperature is relatively easily measured especially by remote means. The stream-function equation allows the establishment of such a relationship as long as other terms are neglected. Since it is not a priori clear that any of these terms are negligible it remains to be seen how well such a model works. In order to verify this technique some field experiments along with perhaps more sophisticated numerical modeling would be in order.

IV. Atmospheric Transformation Modeling

Many of the harmful substances present in an urban air mass are generated in situ through atmospheric transformations resulting from species emitted in the area and its environs reacting with other pollutants or natural species under the action of sunlight. The most notable example of this of course is the production of smog in the Los Angeles basin. Hydrocarbon and nitric oxide, primary pollutants of fossil fuel combustion, are major reactants in the formation of photochemical smog. The formation of oxidant in polluted urban atmospheres occurs via complex free radical chain reactions involving these two pollutants. The chain reactions resulting in the oxidation of both hydrocarbon and nitric oxide are initiated and propagated by sunlight. In order to accurately assess the impact of various control strategies it is necessary to model this complex process.

The EPA has over the past few years developed three photochemical models capable of calculating the oxidant concentration on a day to day basis in the Los Angeles basin. Last year these models were tested against some six days in which comprehensive data were collected. The dynamics of two of these models is different. The model developed by Roth, et al. (3) at Systems Applications is a grid point calculation. The grid covers the whole of the basin and concentrations are calculated for each grid point each increment of time. The model developed by Eschenroeder and Martinez (4) of General Research Corporation and that by Wayne, et al. (13) of Pacific Environmental Services are trajectory models. They consider that a column of air can be defined of roughly 2km. diameter and a depth equal to the mixing layer. This column traverses the city following a trajectory determined from the wind field. Pollutants enter at the bottom of the column, are reacted upon and the oxidant concentration results. Such models offer an advantage in computer resources required over the grid point model but the disadvantages are many. Perhaps the major criticism is really a restriction. Namely the trajectory approach is valid only so long as a coherent parcel of air can be identified and such a concept is meaningful. The general meteorological condition however is for the wind direction to change substantially with height and for turbulence to cause severe mixing. The extent to which a parcel remains intact and indeed to which such a concept is valid has been the subject of a recent field program in the Los Angeles area. The study known as the Los Angeles Reactive Pollutant Program (LARPP) included the following features:

> Tracking of tetroons by radar release of three balloons at same place and time.
>
> Helicopter flights approximately along the centroid at the balloon triplet - vectored by balloon observations. Instrumentation included NO, NO_x, CO, O_3, HC, Methane, Nephelometer, dew point, temperature, etc.
>
> Ground based measurements with instrumented van following approximately under the tetroon triplet.
>
> Lidar measurements to ascertain the depth of the LA mixed layer.

Radiation measurements of the intensity at six sites in LA.

The study under joint funding from EPA and the Coordinating Research Council (CRC) an organization of the American Petroleum Institute and the Society for Automotive Engineering was carried on for about 35 days last September through November. The data which have been collected are being archived by the General Research Corporation. When completed this archive will be available to the public. In order to acquaint interested individuals with the data a symposium and data archive users workshop are being held this November (1974) in Santa Barbara, California.

Our extramural research this past year in transformations has centered on the establishment of a so called second generation photochemical model. SAI, under the direction of Dr. Roth, has been working for the past year on this effort. The various limitations of each modeling methodology were studied and critical comparisons between models were made. Finally a substantial new development of the second generation model has been undertaken. The new development includes the following features:

Subgrid scale considerations - The model now calculates a 2 miles square average value. Neither sources nor receptors are on this scale so special models or methodology are required.

Photochemical mechanism - Current models use a lumped reaction mechanism which is fictitious. A new mechanism which accounts for at least 3 separate classes of hydrocarbons seems to be lumped in a more chemically realistic manner.

Multiday simulations - Current models run from say 0500 until 1600-1800 and thus are unable to calculate the morning (0500) oxidant for example. Improved numerical methods must be introduced to allow such a day-to-day calculation.

Sulfur Atmosphere - Current models do not include sulfur chemistry since Los Angeles has very little SO_2 pollution. This is not, however, the general case and thus the processes must be included.

Our recent inhouse work in atmospheric reactions has centered on two tasks. The first is the development of a useful photochemical-oxidant model. To this end we have begun exploring the possibilities of combining acceptable photochemical transformation parameterizations with simpler meteorological models. Hanna (24) has reported on the use of the box model with a reaction mechanism. We have, in connection with some other concerns to be discussed later, developed a multilevel box model. Dr. Kenneth Demerjian, of our laboratory, is currently investigating various mechanisms as to their suitability for inclusion in such a model. The object of such a development would be an oxidant model with some degree of acceptability yet which could easily and rapidly be exercised for many diverse air quality control regions.

Dr. Demerjian is studying the reaction mechanism which determines the ultimate fate of SO_2 emitted from stationary sources. An indication of the chemistry involved is given in Table 1.

Finally in an attempt to simplify the rather complex SAI model we contracted with Dr. Mizel of Technology Service Corporation to do a so called repromodel. The advantages are substantial in terms of computer time. It is however, necessary to adopt an attitude of total faith in the workings of the SAI model. Further, there is no information in the repromodel once you go beyond (above or below) the data for which the repro was built. It is fair to say that while this is a promising idea in practice we must have substantially more information and validation before we could accept such a model.

V. Diffusion Model Validation and Simplification

For a number of years the air quality modeling community has been fascinated with the techniques for solving diffusion equations. With the emergence of the high speed computer came the realization that hitherto undreamed of complexity could be added to models. We have responded with a proliferation of different methodologies. The modeling community has discussed the pros and cons of assuming solutions to the equations, such as the Gaussian plume and Gaussian puff and integrating over these solutions using various techniques. We have argued the benefits of a grid point model and a trajectory model. Indeed, within the grid point approach discussion has in recent years focused upon what method is used to solve the equation, namely finite differences with their well known associated errors of numerical diffusion (uncentered schemes) or phase (centered schemes), particle in cell methods and spectral techniques. It is now time to reassess the value of the various model types which have been developed. This is the primary purpose of our Regional Air Pollution Study (RAPS).

Three models which will be compared for St. Louis are (1) a Gaussian multiple source diffusion model developed by Geomet (25), (2) a multilevel box model developed inhouse (26) and (3) a three-dimensional finite difference model developed by Shir and Sheih.(27)

This past year Kontnik (26) and Clarke developed a modified box model reported above. It is based upon the assumption that horizontal diffusion can be neglected with respect to vertical diffusion and advection in an urban area. This model essentially moves material along the wind direction, adding the proper amount of vertical mixing. The model was found to be quite sensitive to the depth of the mixing layer. Substantial improvements of correlations between calculations and measurements accrued using realistic (based upon our experiments in St. Louis) values of the mixing depth. Because of the need for an urban mixing depth model, Clarke and McElroy (6) suggested the relationship shown in Figure 3 between mixing depth in the city and the airport (rural) sounding. We still need to collect substantially more data to verify such a model.

One of the problems facing EPA currently is the delineation of long range atmospheric transport of pollutants. By long range we mean the transport from one air quality control region (city) to another. City A is learning that when it cleans up its sources City B which is upwind contributes unacceptably high levels of background pollution back to A. Clarke has developed a trajectory model, based upon normally available weather data, to calculate the effects of such long range transport. We are now validating the model on meteorological data.

An associated, if somewhat opposite, problem is determining the nature of pollution dispersion close to the source. This is particularly significant for determining the impact of highways on air quality. While we currently have a working highway model, based on a line source Gaussian process, the dispersion coefficients used are quite uncertain, closer than 100m from the source. In order to develop the necessary data, we have funded a measurement program. An auto able to release fluorescent particles is driven along a highway. Off the highway is instrumented with meteorology towers and a small network of FP instruments. Close-in diffusion coefficients are determined from the data. In a related study a group from the State University of New York and Brookhaven National Laboratory (Drs. Ogden and Rayner) have performed extensive studies of the dispersion of pollen near the sources.

Finally, our major effort currently is in trying to develop a model testing and validation plan for the RAPS. Our ideas have been described in more detail elsewhere. (27-29)

VI Physical Model Program

Our physical modeling program has been well described elsewhere. (30) A point I wish to make here is that our research is very much intertwined with the wind tunnel. We hope the major use of the tunnel will be for research. In particular, we would like to model small (say, 2km square) urban areas with the wind tunnel and develop information on much finer scales than could ever be measured in the city or could ever be calculated numerically. Eventually, we would hope to do "side-by-side" wind tunnel and real atmosphere comparison experiments.

We have recently contracted for the construction of a water channel.

The advantage of such a facility is that any realistic stable stratification can be achieved by mixing water with varying salt content and hence varying density. Once the density gradient is established a model is towed (upside down) along the surface of the tank.

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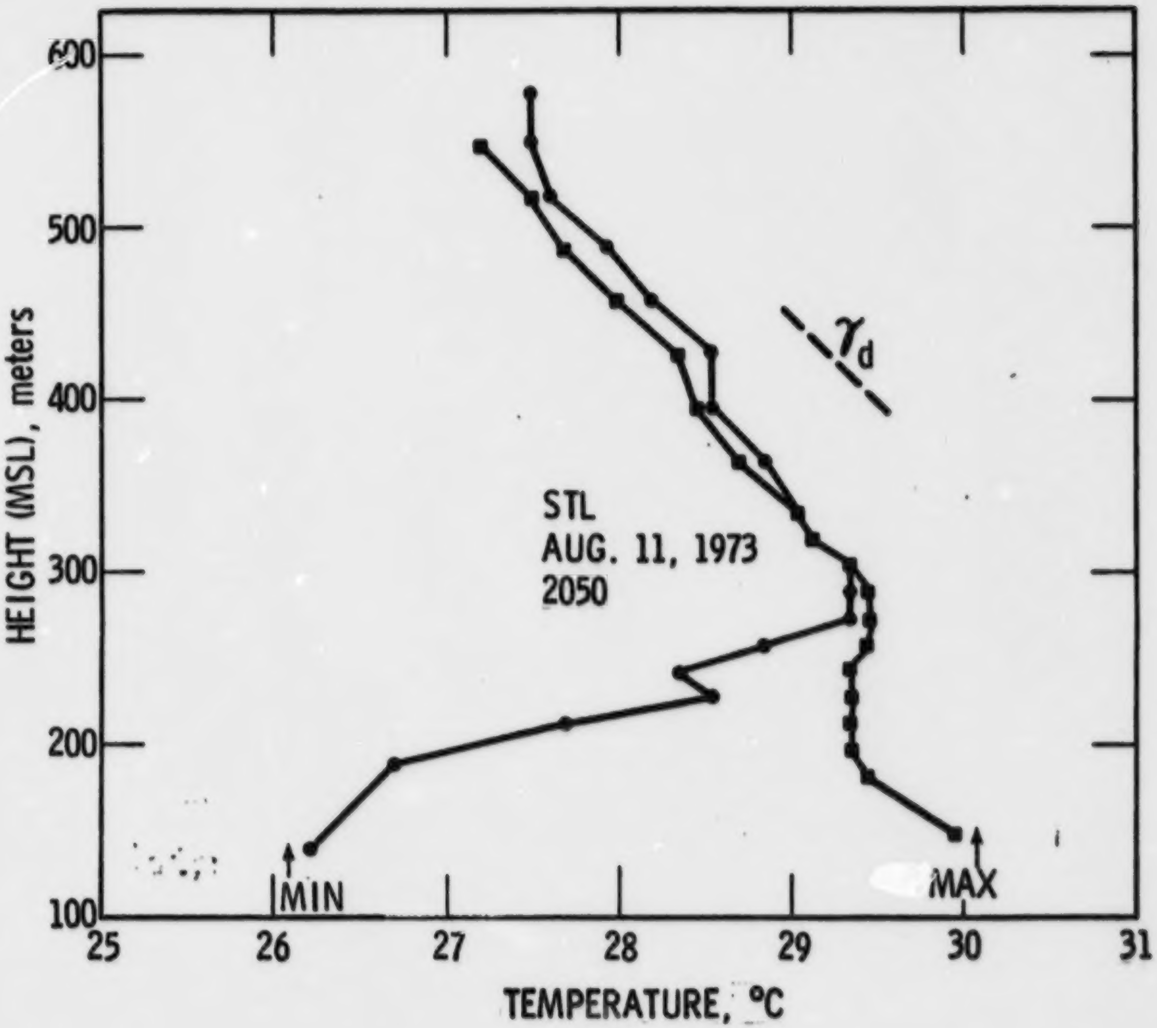
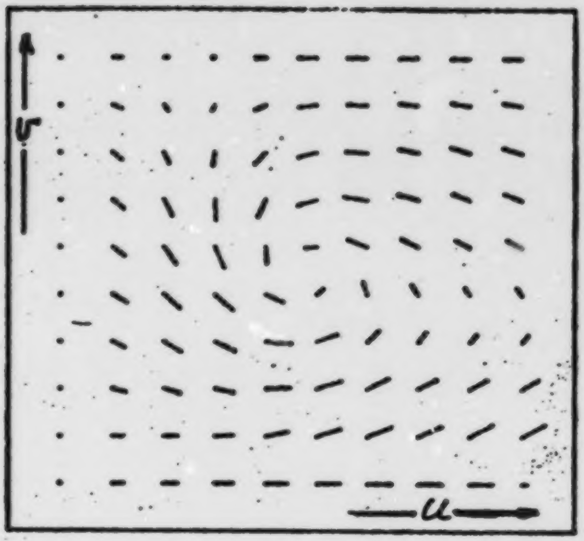
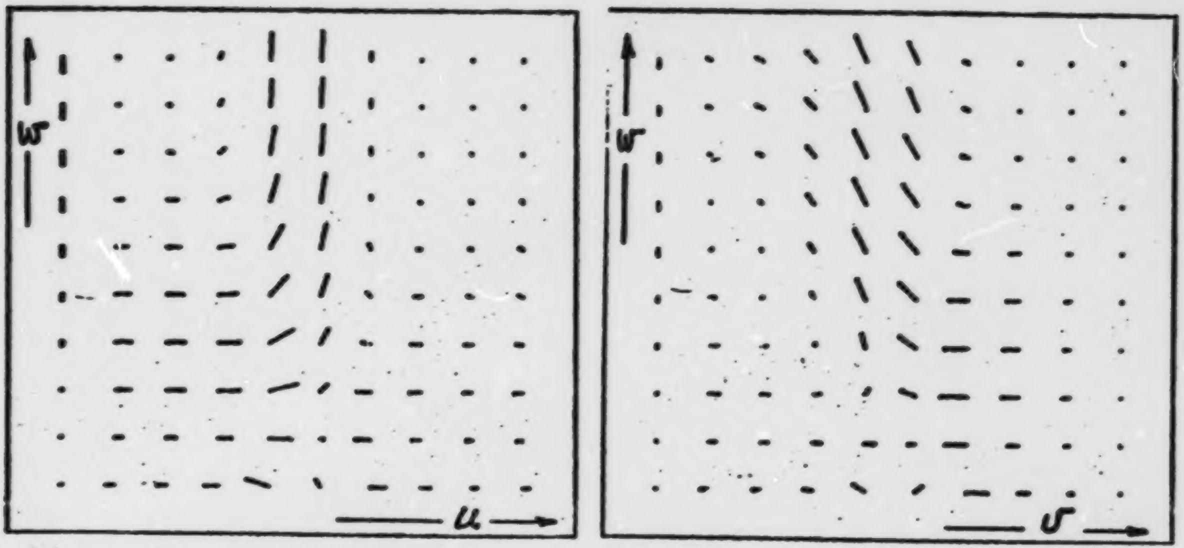


Figure 1. Urban (■) Rural (●) Temperature Contrast (6)



(a) Horizontal velocity field (half-way up the box)



(b) Vertical slice displaying U & W vectors (halfway in the box)

(c) Vertical slice displaying V & W vectors (halfway in the box)

Figure 2. Preliminary Flow Field From WATPC. Steady state flow field resulting from a three-dimensional numerical model (using techniques developed in (31)). Central portion of grid is heated causing a "thermal low" which generates the circulation.

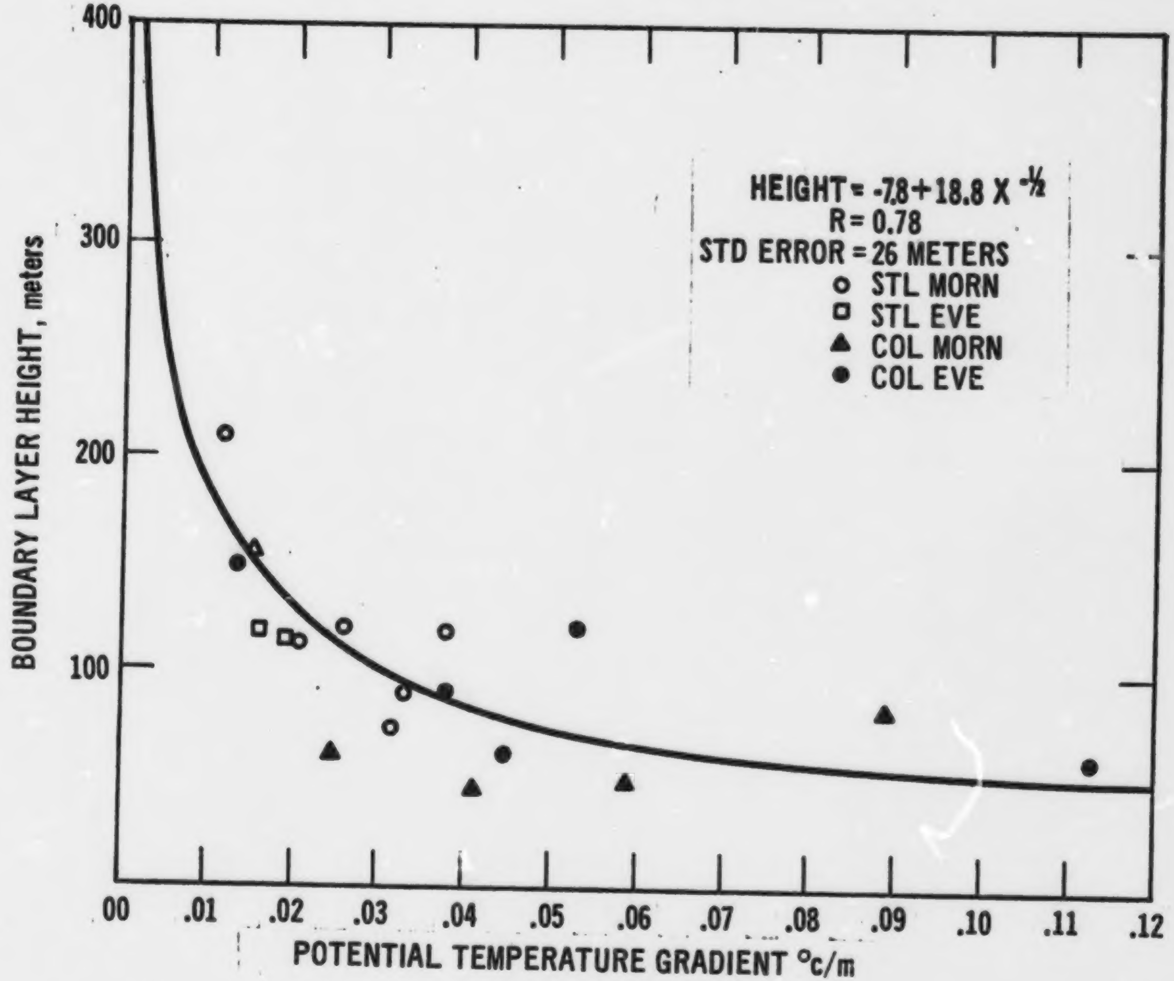
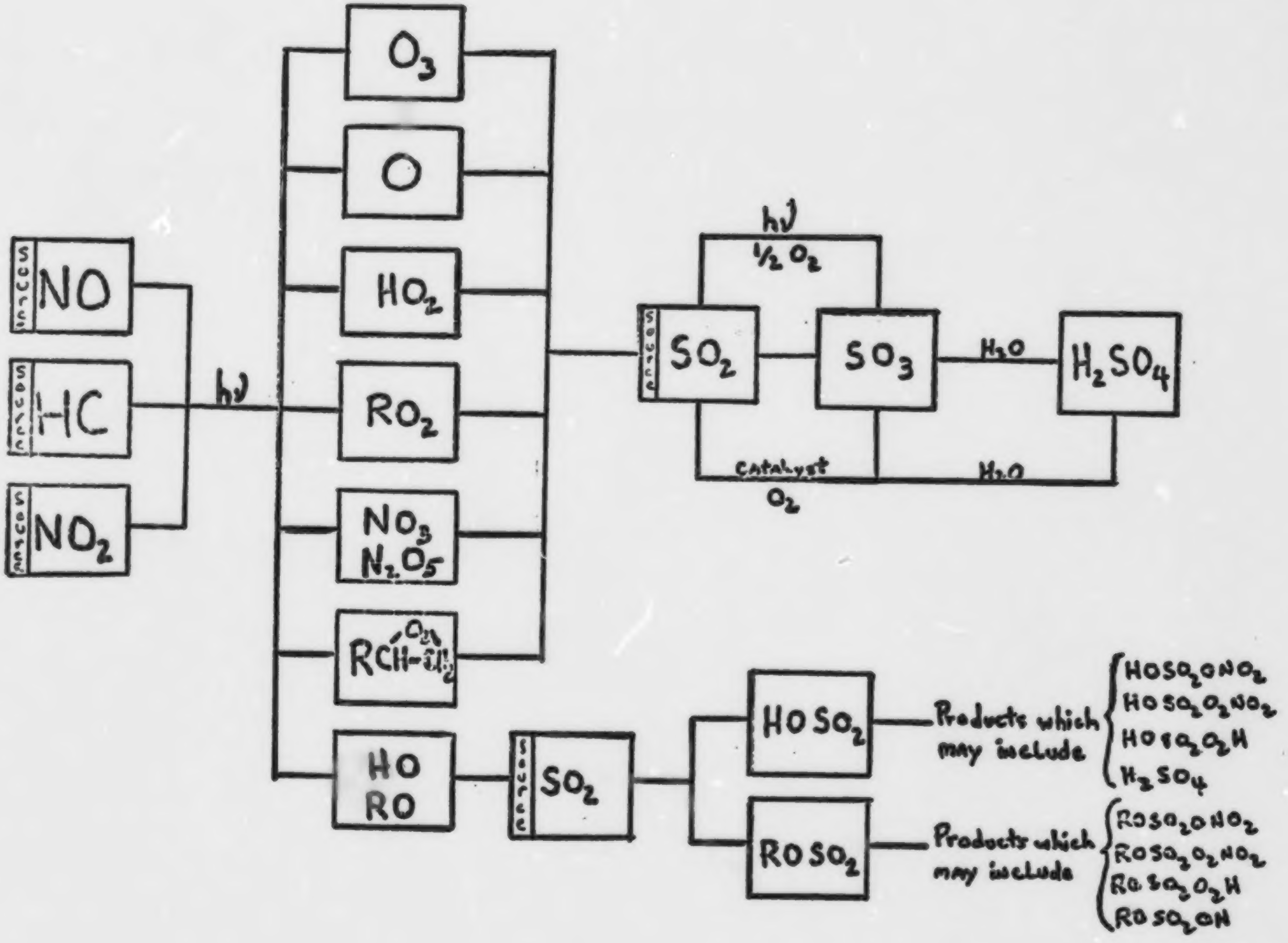


Figure 3. Depth of the Urban Modified Layer as a Function of Suburban Soundings (6)

Table 1


source
NO
source
HC
source
NO_2
hν
O_3
O
HO_2
RO_2
NO_3
N_2O_5
RCH-
HO
RO
source
SO_2
hν
$1/2\ O_2$
SO_3
H_2O
H_2SO_4
catalyst
O_2
H_2O
source
SO_2
$HOSO_2$
Products which may include
$HOSO_2ONO_2$
$HOSO_2O_2NO_2$
$HOSO_2O_2H$
H_2SO_4
$ROSO_2$
Products which may include
$ROSO_2ONO_2$
$ROSO_2O_2NO_2$
$ROSO_2O_2H$
$ROSO_2OH$

Chapter 34

ASSESSMENT OF THE VALIDITY OF AIRSHED MODELS

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

ASSESSMENT OF THE VALIDITY OF AIRSHED MODELS

At the Second Meeting of the Expert Panel on Air Pollution Modeling (Paris--July 1971), F. L. Worley, Jr. presented a report detailing progress in modeling photochemical smog. Largely supported by the U.S. Environmental Protection Agency (EPA), model development in this field was initiated primarily because existing models, most prominently the Gaussian dispersion model, were unsuitable for representing the combined transport and reaction processes that take place in the atmosphere. Photochemical models that have been developed to date are based on the species continuity equations,*

$$\frac{\partial c_i}{\partial t} + u\frac{\partial c_i}{\partial x} + v\frac{\partial c_i}{\partial y} + w\frac{\partial c_i}{\partial z} = \frac{\partial}{\partial x}\left(K_H \frac{\partial c_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(K_H \frac{\partial c_i}{\partial y}\right) + \frac{\partial}{\partial z}\left(K_V \frac{\partial c_i}{\partial z}\right) + S_i + R_i(c_1, c_2, \ldots.) \qquad i = 1, 2, \ldots, p \quad , \qquad (1)$$

where

K_H, K_V = horizontal and vertical turbulent eddy diffusivities

S_i = rate of emissions of species i from elevated sources

R_i = rate of production of species i through chemical reaction

c_i = time and space averaged concentration of species i.

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* The Gaussian is, of course, a solution of the species continuity equation under a rather restrictive set of assumptions.

It is assumed in these models that:

(1) K-theory applies.

(2) Concentration fluctuations (and thus their effect on reaction rates) can be neglected.

(3) Molecular diffusion can be neglected.

(4) Air is incompressible.

However, the following assumptions, required for the Gaussian formulation, are not necessary for the photochemical models:

(1) The concentration field is invariant with time.

(2) The wind velocity is constant, and the vertical component of the wind w is zero.

(3) K_V is independent of z, and K_H is independent of x and y.

(4) Pollutant species are nonreactive.

Two major types of approaches have evolved in the development of short term photochemical models* capable of predicting the spatial and temporal variations in air quality over the course of a day or more: trajectory models and grid models. Trajectory models are based on the notion of computing concentrations in a moving column (or parcel) of air as it traverses an airshed. The column is usually assumed to be of fixed cross-sectional area and variable height, with the top of the column being at an elevation equal to that of the local inversion base or the upper boundary of the well-mixed layer. Two models of this type have been developed under EPA contract and have been discussed in some detail by Worley (1971) [see Eschenroeder and Martinez (1972) and Wayne et al. (1973)]. Grid models, in contrast, are based on dividing the modeling region in a discretized, three-dimensional grid and solving Eq. (1) using an appropriate numerical solution technique. A model of this type has also been developed under EPA auspices [Roth et al. (1971), Reynolds et al. (1973)].

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* Although they are called photochemical models, models based on Eq. (1) can be applied equally well for both inert and reactive pollutants.

At the Fourth Meeting of the Expert Panel on Air Pollution Modeling, D. B. Turner and R. F. Lee (1973) discussed the advantages and disadvantages of trajectory and grid models. One distinction of particular interest is the fact that grid models predict concentrations over the full modeling region for any prescribed time interval, whereas trajectory models calculate concentration histories only along the particular path followed. Thus, a large number of trajectory calculations must be carried out to predict a full concentration field. However, both the computing time and the storage requirements associated with grid-based simulations are far greater than those associated with trajectory calculations. [See Seinfeld et al. (1972) for a more complete discussion of this topic.]

Despite the fact that the strengths and shortcomings of grid and trajectory models are clearly understood and the assumptions upon which they are based are well known, the range of validity of these models has never been formally established. Such knowledge has been needed for some time to aid the selection of appropriate modeling techniques for particular applications. Because of this need, we undertook a study to assess the validity and range of validity of grid and trajectory models, restricting our effort to an evaluation of those photochemical models developed under EPA auspices. The remainder of this paper is devoted to a brief presentation of the results of that study. Full details have been reported by Liu et al.(1974).

The two trajectory models that have been developed are based on the following assumptions, over and above those stated earlier:

(1) Neglect of horizontal diffusion

(2) Neglect of the vertical component of the wind ($w = o$)

(3) Neglect of wind shear ($\partial u/\partial z = \partial v/\partial z = o$).

In addition, it is assumed in one of the two models that the atmosphere is well mixed in the vertical. In contrast, none of these assumptions are made in the grid formulation. However, it is assumed that the discretized form of Eq. (1) is a valid approximation to the differential form shown and, thus, that errors generated by numerically solving the discretized equation can be neglected. Our evaluation is limited to a consideration of (1) the three basic assumptions on which the trajectory concept is founded, as derived from the diffusion equation, and (2) the effect of discretization on grid solutions.

It was decided at the outset to use the diffusion equation [Eq. (1)]--rather than a more fundamental form of mass balance for species--as the standard for all evaluative comparisons. However, for such comparisons to be meaningful, the "base" solutions to this equation must be exact and, thus, analytical rather than numerical. This restriction precluded consideration of the full, unrestricted, three-dimensional, time-dependent problem. Rather, special restricted, two-dimensional (x and z), time-varying formulations were considered--formulations that clearly allowed an evaluation of the effect of each of the three trajectory model assumptions when solutions of the trajectory model and diffusion equation were compared. Moreover, since meteorological variables were of primary concern, chemical reactions and volume sources were not considered. Thus, the following equation served as the standard against which comparisons were made:

$$\frac{\partial c}{\partial t} + u\frac{\partial c}{\partial x} + w\frac{\partial c}{\partial z} = \frac{\partial}{\partial x}\left(K_H\frac{\partial c}{\partial x}\right) + \frac{\partial}{\partial z}\left(K_V\frac{\partial c}{\partial z}\right) \quad . \qquad (2)$$

In the evaluation of the trajectory model, three specific formulations of Eq. (2) were considered, each for the assessment of a particular assumption.

(1) Horizontal diffusion--the application of Eq. (2) for a continuous, ground level area source and for a cross section of a realistic, urban-type source distribution where

u = constant

w = 0

$K_z = K_1\left(\frac{z}{z_1}\right)^n$

K_H = constant.

(2) Vertical transport--the application of Eq. (2) for a continuous, ground level, crosswind line source

where

$$u = (u_1 - ax)\left(\frac{z}{z_1}\right)^m$$

$$w = \frac{az}{m+1}\left(\frac{z}{z_1}\right)^m$$

$$K_z = K_1\left(\frac{z}{z_1}\right)^n$$

$$K_H = 0.$$

In this case, the parcel velocity U for the trajectory model is taken to be $u_1 - ax$.

(3) Wind shear--the application of Eq. (2) for a simple, continuous, crosswind line source and for a cross section of a realistic, urban-type source distribution

where

$$u = u_1\left(\frac{z}{z_1}\right)^m$$

$$w = 0$$

$$K_z = K_1\left(\frac{z}{z_1}\right)^n$$

$$K_H = 0.$$

Both analytical and trajectory model solutions were obtained and compared for ranges of values of meteorological parameters that are typically observed in urban areas.

The results of these comparisons can be summarized as follows. The effect of neglecting horizontal diffusion, even under conditions most unfavorable to the validity of the assumption, is small--always less than 10 percent. The effect of neglecting the vertical wind component is more interesting and more complex; it is best shown in plots such as Figure 1 of γ versus ψ for varying values of ζ, where

$$\gamma = \frac{\text{concentration predicted using the trajectory model}}{\text{concentration predicted using an analytical solution to Eq. (2)}}$$

$$\psi = \text{nondimensional horizontal distance} = \frac{u_1 - ax}{u_1 - ax_s}$$

$$\zeta = \text{nondimensional reference height} = \frac{z_1}{\sqrt{K_1/a}} .$$

If $n = 0$ or $m = 1$, γ is independent of ζ. In either case, however, the trajectory model always overpredicts (i.e., $\gamma > 1$); also $\gamma - 1$ increases with ψ. Furthermore, $\gamma - 1$ increases as n decreases and as m increases. For general values of n and m, the ratio γ depends also on the choice of the reference height ζ; in this case the trajectory model predictions increase with a decrease in ζ. The ratio γ, however, always increases with ψ, indicating a predicted accumulation of pollutants due to the lack of vertical transport in the trajectory model. The most significant general conclusion to be drawn from the analysis of the neglect of the vertical wind component is that, for meteorological conditions typical of those observed in urban environments,* the value of γ can vary greatly

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* That is, strong convergence near the center of a city due to the urban heat island effect. Ackerman (1974) estimated that the strength of this convergence in St. Louis is 3×10^{-4} sec^{-1}.

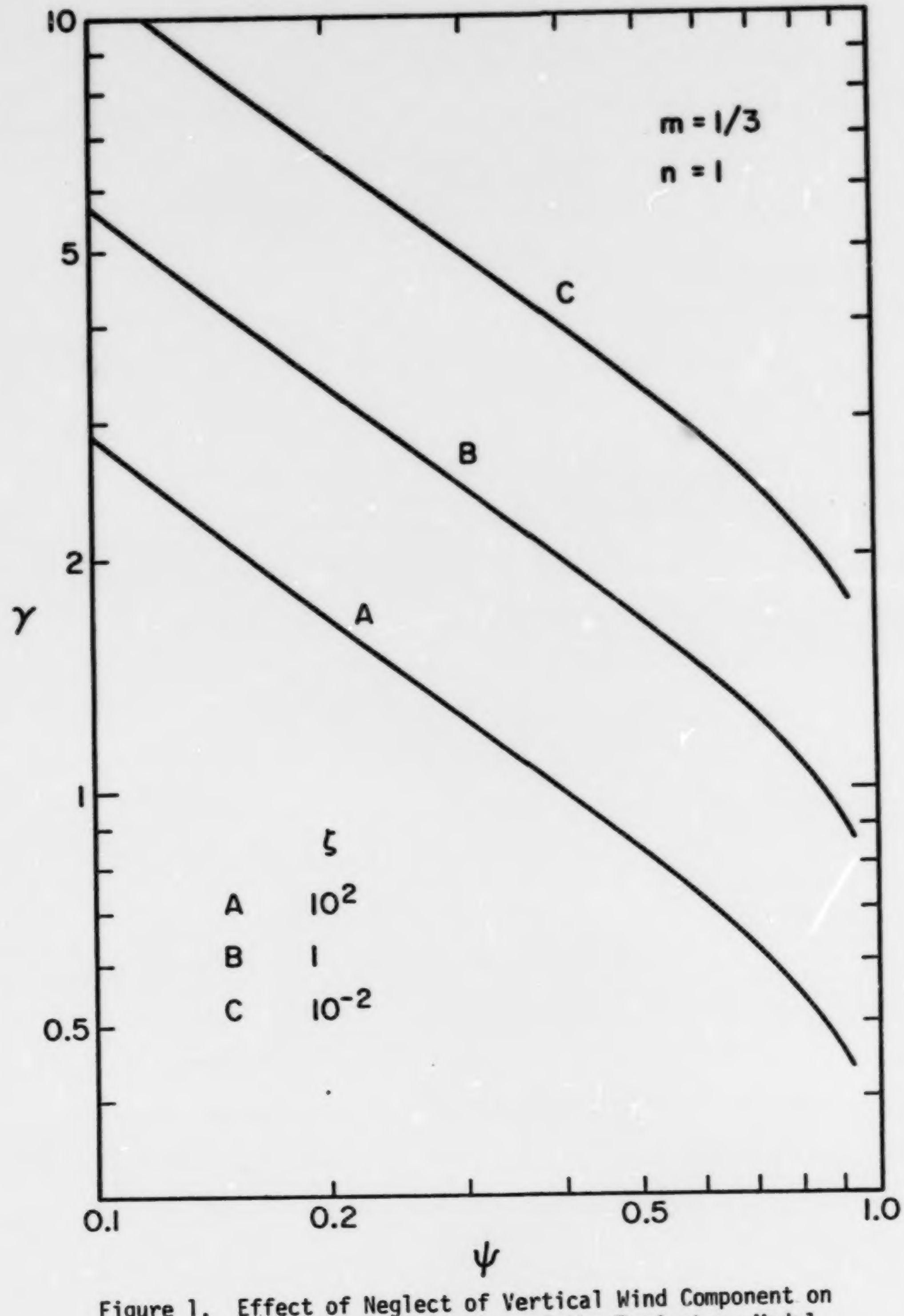

Figure 1. Effect of Neglect of Vertical Wind Component on Accuracy of Prediction of the Trajectory Model

(i.e., by an order of magnitude), particularly as ψ becomes large. Thus, except for the case of a vanishing vertical component of the wind (i.e., $a \to 0$ and $\psi \to 1$), considerable care should be exercised in the application of existing trajectory models. However, although the vertical component of the wind is neglected in the trajectory models developed to date, the concept of such a model has no fundamental limitation prohibiting the inclusion of this component. Rather, the added computational burden that the inclusion of w creates in part negates the attractiveness of the trajectory approach.

Finally, we consider the third assumption, neglect of wind shear, a variable that trajectory models do not presently include and cannot accommodate. Results presented in the form of plots of γ versus x for meteorological and emission conditions typical of urban environments indicate that trajectory models can overpredict ground level concentrations by 50 percent or more. For instance, for

$$u_1 = 1.5 \text{ m/sec}$$

$$z_1 = 10 \text{ m}$$

$$K_1 = 1 \text{ m}^2/\text{sec}$$

$$\Delta x = 3000 \text{ m},$$

the values represented by the triangles in Figures 2 and 3 apply. For a continuous line source and values of n and m of $0.2 < m < 0.4$ and $n \simeq 1$, respectively (values typically observed in cities), errors are also of the

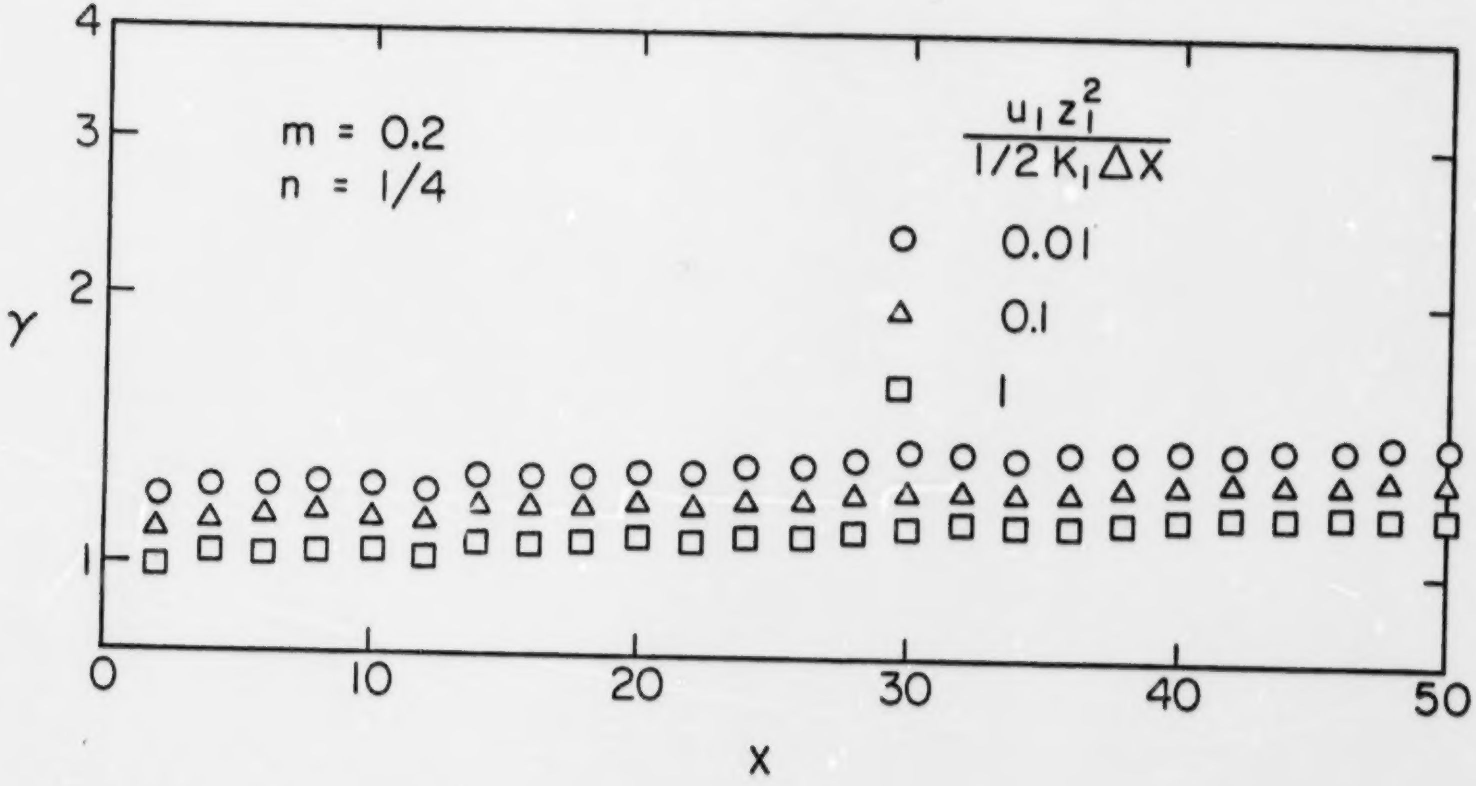

Figure 2. Effect of Neglect of Wind Shear on Accuracy of Prediction of the Trajectory Model (m = 0.2, n = 0.25)

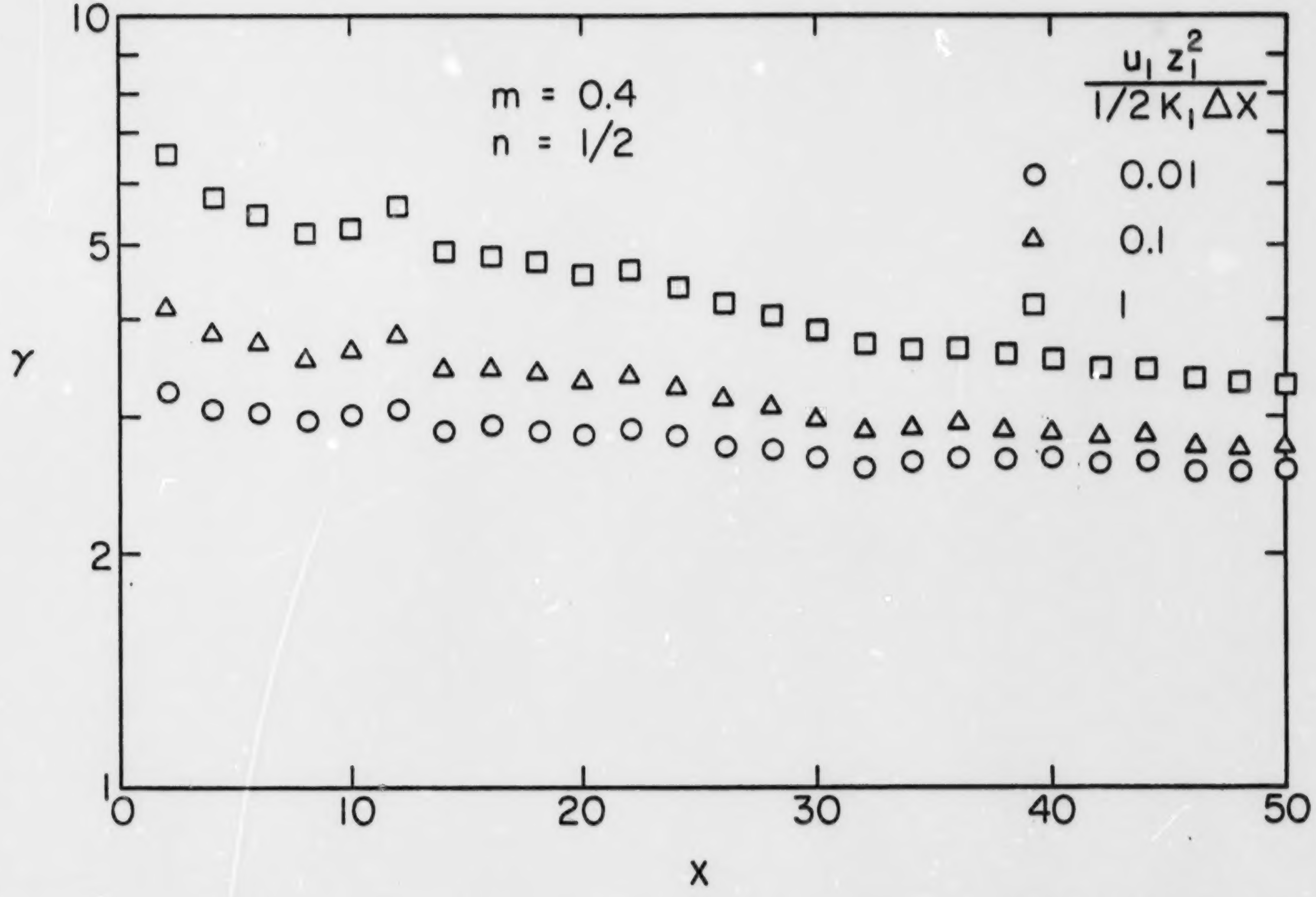

Figure 3. Effect of Neglect of Wind Shear on Accuracy of Prediction of the Trajectory Model (m = 0.4, n = 0.5)

order of 50 percent. Clearly, the neglect of shear can have the effect of significantly degrading the accuracy of predictions.

We noted earlier that errors introduced by discretization are the sole source of the disparity between "exact" solutions of the diffusion equations and numerical solutions on a grid. For the grid model developed by Roth et al.(1971), the solution is carried out using the method of fractional steps for a 50 by 50 mile region, with each grid square being 2 miles on a side. To determine the magnitude of errors introduced for realistic emissions and meteorological conditions, we adopted the same assessment procedure as was employed for the evaluation of the trajectory model; i.e., we solved a two-dimensional (crosswind), time-dependent formulation both analytically and by means of numerical integration and compared results. As before, Eq. (2) served as the standard, in this case with u, K_H, and K_V being held constant (at realistic atmospheric levels) and with w set equal to zero. Both first and second order differencing schemes were investigated. (A second order scheme is employed in the actual model.) As expected, the first order method introduced significantly larger errors than the second. Moreover, the errors as a function of time exhibited wave-like variations that increase in amplitude and phase angle as the simulation time increases. For the second order procedure, at the end of a nine hour simulation, errors of ± 20 percent were observed for the smooth emissions pattern, and errors of ± 50 percent were observed for the realistic emissions pattern. Clearly, extreme caution must be exercised in the selection of a numerical scheme, particularly if long simulation times are expected. We are now exploring the use of at least two methods that have the potential for reducing error propagation substantially: the "material-preserving" procedure developed by Egan and Mahoney (1972) and the spectral method suggested by Orszag (1970) and Orszag and Israeli (1974). The preferred method will then be incorporated in the model, and a full error analysis will be reported.

The *qualitative* results of this study, which are summarized in Table 1, are by no means unexpected. However, the *quantitative* results* contribute substantially to the ability of the potential user to decide on an informed basis if, in fact, one or another type of model can be meaningfully applied under a prevailing set of meteorological and emission conditions. In short, the range of validity of grid and trajectory models can now be accurately assessed.

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* See Liu, et al. (1974) for a complete presentation of results.

Table 1. Qualitative Assessment of the Validity of Grid and Trajectory Models

Model	Assumption	Magnitude of Errors Introduced (for typical urban conditions)	Possibility of Rectification
TRAJECTORY	Neglect of horizontal diffusion	Slight	Rectification not needed
	Neglect of vertical component of wind	Can be substantial	Excellent (but at the expense of longer computing times and more data handling)
	Neglect of wind shear	Can be substantial	None
GRID	Neglect of errors introduced through discretization	Substantial	Good (incorporation of more suitable techniques)

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Chapter 35

EMPIRICAL APPROACHES TO AIR QUALITY AND METEOROLOGICAL MODELING

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

EMPIRICAL APPROACHES
TO AIR QUALITY AND METEOROLOGICAL MODELING

W. S. Meisel

INTRODUCTION

There has been a recent increase in interest in the use of empirical approaches to the analysis of air quality problems. This paper will review the sources of this increased interest, some possible uses of empirical approaches, difficulties associated with empirical analysis of air quality data, and approaches to overcoming those difficulties. The paper will conclude with an outline of a study of an empirical approach to the analysis of data arising from a computer model based on physical principles--an example of the complementary nature of physical and empirical approaches.

MOTIVATION FOR INCREASED USE OF EMPIRICAL APPROACHES

Three of the major reasons for increased interest in the use of empirical approaches in air quality analysis are the following:

(1) More and better data are available for analysis;

(2) Improved methodology for solving the type of data analysis problem which most often represents itself in air quality applications has been developed over the past few years; and

(3) Combinations of empirical approaches and approaches based upon physical reasoning may lead to better problem solutions than either approach alone.

Improved data bases are a result both of a number of measurement programs and of a longer history of data collection.

The state-of-the-art in empirical analysis has until recent years been such that it had only limited applicability to air quality problems.

The source of this limitation was the large number of variables which affect meteorology and air quality. Hence, a large number of cases are required to reflect the full diversity of those variables affecting the outcome of interest. To be specific, suppose there were ten variables measured, all of which might have an effect on some air quality outcome to be predicted. If only three values of each variable were allowed, the number of cases required to represent all combinations of values of the ten variables is 3^{10}, or 59049. This is a somewhat exaggerated example of the "curse of dimensionality"; a more lengthy discussion of the relation between the number of variables and required sample size can be found elsewhere[1]. The point of this brief discussion is that the majority of air quality and meteorological data analysis applications involve a large number of variables which may potentially affect the outcome in question; this characteristic in turn implies that the sample size, i.e., the number of cases measured, will tend to be small relative to the diversity possible in the independent variables. We will thus in general be dealing with a small-sample, multivariate data analysis problem -- a difficult and non-classical category of problems. The likelihood that the problem will require a nonlinear solution compounds the difficulty. Recent attention to nonlinear small-sample, multivariate data analysis techniques, however, has made it possible to approach these problems with greater confidence and has motivated interest in the application of such approaches in the air quality field.

DIFFICULTIES ASSOCIATED WITH EMPIRICAL ANALYSIS OF AIR QUALITY DATA

Clearly empirical approaches are not without difficulties:

(1) Appropriate data from whatever source must be available.

(2) The curse of dimensionality, as mentioned, imposes requirements on sample size because of the typically large number of independent factors affecting the outcome of interest. This often requires a much larger number of cases than is intuitively obvious.

(3) An empirical analysis can be limited in terms of generality and transferability. For example, a study done on photochemical smog using data collected in Los Angeles may not be applicable to other cities.

OVERCOMING THE DIFFICULTIES

There are several ways in which the indicated problems can be approached successfully:

(1) One might simply limit one's objectives when appropriate. If, for example, one analyzes photochemical smog data from Los Angeles, the detailed quantitative model may not be transferable, but the qualitative conclusions may be broadly applicable or may aid the development of physically based models.

(2) An empirical analysis (as compared with the development of a physical model) is a relatively rapid and inexpensive procedure; hence, one can often repeat empirical analyses as easily as one can calibrate, modify, or initialize physical models for new locations.

The third motivation for the use of empirical approaches, the possibility of synergism between empirical and physical approaches, forms a part of the discussion of the next section.

THE USES OF EMPIRICAL APPROACHES

Empirical approaches can be employed in some conventional--and some unconventional--ways:

- Direct analysis of measured data
- The analysis of data arising from physically based mathematical models
- Combined empirical/physical models.

We shall discuss these in turn.

Direct Analysis of Measured Data

Given an appropriate set of data, a quantitative model relating input (independent) variables to an output (dependent) variable can be constructed by a number of techniques. One of the best known statistical/empirical models in the air quality field uses pollutant concentration data with one averaging period to predict pollutant concentration for another averaging period[2,3]. It should also be noted that the intent of such an empirical analysis may be not only the creation of a quantitative model, but the extraction of the qualitative implications of the data, e.g., the relative effect of one variable versus another.

The Analysis of Data from Models Based upon Physical Principles

The empirical analysis of data arising from exercising a physically based mathematical model has been termed repro-modeling[4]. Motivation for analyzing data arising from a model is similar to that in analyzing direct measurement data: (1) One may wish to know the general qualitative implications of the model and to explore those implications in a systematic manner; and (2) one may wish to have a direct quantitative model of the model or of an aspect of the model which can be used more easily and inexpensively for planning purposes. Other purposes are related to validating and improving the physically based model: If the implications of the model can be explored fully, characteristics which are physically unreasonable can lead to the discovery of programming errors or appropriate modifications of the model. A repro-modeling study was done on a photochemical pollution model for the U.S. Environmental Protection Agency[5]; the approach and its results are outlined briefly at the end of this paper.

Combined Empirical/Physical Models

Many difficulties with physical and empirical models can be overcome by a hybrid approach. Many physical models could benefit from empirical components explaining the more stationary processes involved; these processes may be difficult to analyze through pure deductive means. On the other hand, non-stationary aspects of empirical models could be modeled from physical principles in order to enhance the generality of an empirical model. Another form of interaction between physical and empirical modeling approaches is when the independent variables are combined into a summarizing quantity through physical principles and intuition (e.g., summarizing relevant meteorological variables into a measure of atmospheric stability). Similarly, one could use physical knowledge and intuition to suggest the form of an empirical model in order to reduce the number of parameters to be determined empirically.

(3) Difficulties such as those discussed may often be overcome, as in any technical problem, by creativity in problem formulation and solution. Such creativity takes a certain amount of time and effort; empirical analysis is no exception. Hence, a problem which may not appear to be amenable to empirical analysis might indeed be solved, given sufficient effort. For example, it has been at times suggested that an empirical analysis cannot produce detailed spatial distributions of pollutant levels, as produced by many physically based models. However, orthonormal functions can be used to express a complex distribution function by a minimal number of coefficients of an expansion, and those coefficients predicted; this approach has been applied to meteorological problems in at least one form[6].

AN APPLICATION EXAMPLE

Let us outline an example of empirical analysis which is unconventional in that the data arises from a mathematical model created from basic physical and chemical principles.

Several physical models which simulate the impact of emissions and meteorology on the creation and dispersion of photochemical smog have been developed. Characteristics of most of these models are that they are highly computational and require a great deal of input data; hence, it is generally difficult to systematically explore the implications of the models or to use them in a planning context where many model runs are required. The study outlined here explored "repro-modeling," the analysis and replication of the input/output characteristics of the model, as a means of meeting these objectives.[5] A study of the application of repro-modeling to a model developed by Systems Applications Incorporated for the Los Angeles Basin[7] is described. The major objectives of the study were threefold: (1) a feasibility test of the repro-modeling approach; (2) a limited interpretation of the implications of the model; and (3) an efficient repro-model program which duplicates input/output relationships of the original model. The repro-model developed was designed for a particular application (transportation emission control policy evaluation).

The study reported had limited objectives and should be interpreted in that light. Limitations on the generality of the results include the following: (a) the original model is calibrated for Los Angeles and the meteorology was fixed; (b) not all aspects of the original model are exercised; and (c) relationships implied by the original model are valid aids for policy design only to the extent that the model represents reality.

Figure 1 illustrates the differences between the repro-model and the original model. The five aggregate input variables were

$MSNO_x$ = Mobile source emissions of oxides of nitrogen
MSHC = Mobile source emissions of hydrocarbons
FSHC = Fixed source emissions of hydrocarbons
$ICNO_x$ = Initial/boundary conditions on oxides of nitrogen
ICHC = Initial/boundary conditions on hydrocarbons.

All variables are expressed as a percentage of their values on a fixed nominal day; e.g., MSCHC = 80 corresponds to reducing mobile source

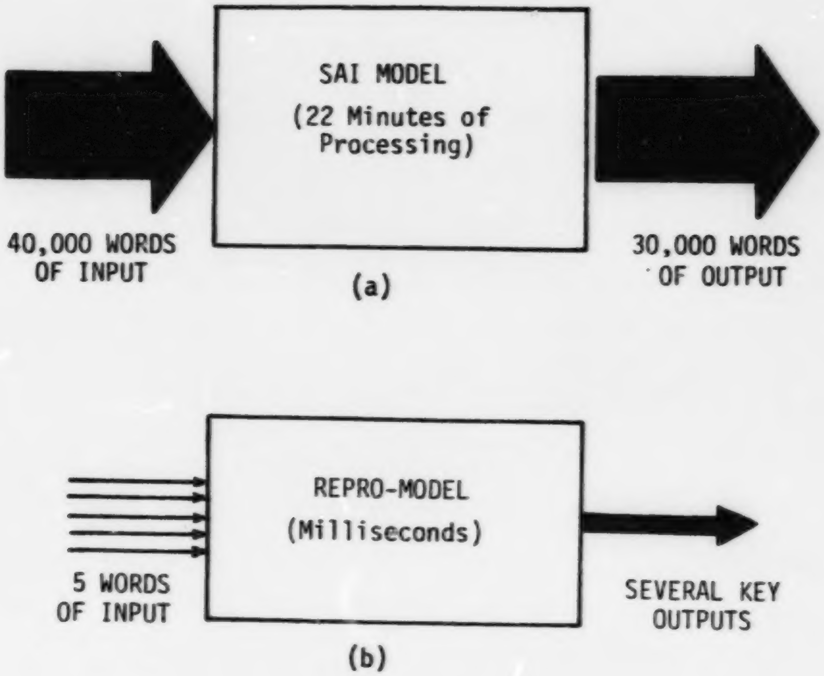
SAI MODEL
(22 Minutes of Processing)
40,000 WORDS OF INPUT
30,000 WORDS OF OUTPUT
(a)
REPRO-MODEL
(Milliseconds)
5 WORDS OF INPUT
SEVERAL KEY OUTPUTS
(b)

FIGURE 1

INPUT-OUTPUT STRUCTURE OF THE ORIGINAL MODEL AND THE REPRO-MODEL

hydrocarbon emissions to 80% of their level on the nominal day, i.e., a 20% reduction.

Using the results of 90 runs of the original model, the level of oxidant and NO_2 resulting from a given choice of values of the five independent variables was modeled empirically at several locations in the

Los Angeles Basin and for the peak level of oxidant irrespective of location. All the models produced outputs which were essentially identical to those of the original model (with typical RMS errors of 0.005 parts per million), but in milliseconds of computer time rather than in 22 minutes. For example, the peak value of oxidant is given accurately by

$$\text{OXIDANT (pphm)} = 0.067\cdot\text{MSNO}_x + 0.342\cdot\text{MSHC} + 0.122\cdot\text{FSHC} + 0.097\cdot\text{ICNO}_x + 0.237\cdot\text{ICHC} - 41.6, \tag{1}$$

when the above equation yields OXIDANT $\geq$ 6.9 pphm. If not,

$$\text{OXIDANT} = -0.005\cdot\text{MSNO}_x + 0.003\cdot\text{MSHC} - 0.001\cdot\text{FSHC} + 0.005\cdot\text{ICNO}_x + 0.001\cdot\text{ICHC} + 6.9 \quad . \tag{2}$$

For example, setting all variables at 100% yields 45 pphm oxidant, which is indeed the peak predicted by the original model for the nominal day.

Let us examine equation (1), corresponding to the higher pollution case. It is easy to see from this equation that mobile source NO_x and initial conditions for NO_x have little effect on the oxidant level. Reducing both variables by 20% will reduce the oxidant level by only 3 pphm (a 7% reduction). On the other hand, the hydrocarbon variables have the predominant effect; reducing MSHC and ICHC by 20% (and leaving fixed sources unchanged) reduces the peak by 12 pphm (a 27% reduction). Hence, the oxidant level at the peak is dominated by hydrocarbon emissions.

The effect of the fixed source hydrocarbon variable is approximately one-third that of mobile source hydrocarbons (by the ratio of their coefficients), indicating that, while mobile sources have the predominant effect as usually assumed, reductions in fixed source emissions can have a significant impact.

A final point can be extracted from equation (1): assumptions regarding the levels of initial and boundary conditions have a major impact on model output. The coefficient of ICHC is comparable with the coefficient of MSHC and dominates that of FSHC; the coefficient of $ICNO_x$ is comparable with that of $MSNO_x$. Since initial and boundary conditions can be predicted only with a great deal of uncertainty, this uncertainty should be reflected in model use. For example, a change of ±20% in initial/boundary condition assumptions for the case where all variables equal 100% would yield an estimate of 45 pphm ± 7 pphm.

Making some reasonable assumptions, equation (1) can be rewritten to obtain a form similar to the "rollback" model:

$$\%\ \text{REDUCTION in } O_3 = -1.56 \cdot \text{MSHC} - 0.28 \cdot \text{MSNO}_x + 184 \quad . \qquad (3)$$

When $MSNO_x$ and MSHC are both set at 100, the percentage reduction in oxidant is, of course, zero. We see that this simple model predicts a 1.6% reduction in oxidant concentration for each 1% decrease in the hydrocarbon emissions variable and a 0.3% reduction in oxidant concentration for each 1% decrease in the NO_x emissions variable. This linear equation holds up to about an 80% reduction.

This type of empirical analysis can considerably broaden the utility of a physically based model.

CONCLUSION

Empirical/statistical approaches in air quality and meteorological applications have received increased attention recently due to the increased availability and quality of data and to improved data analysis methodology for the nonlinear, small-sample, multivariate case. While there can be many difficulties in an empirical analysis, many can be overcome by creative problem formulation and solution. One major source of creative solutions is attention to the possibilities of combining empirical and physically based approaches.

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Chapter 36

DISPERSION FROM TALL STACKS

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
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DISPERSION FROM TALL STACKS

(First and Preliminary Report)

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I. Introduction

During a discussion on model validation problems with several members of EPA, Meteorology Laboratory, it turned out that to the best of knowledge no validation on the basis of a comparison of concentration frequency distribution, had yet been demonstrated for the classical problem of the single elevated point source. The point was made that it is not very useful to try to validate urban air pollution models where there is a mixture of large and small point sources as well as area sources, unless we know that large single point sources are modeled in a satisfactory manner. This is especially true for most of the larger cities where large single sources, such as power plants or chemical factories, are contributing to the concentration field to a great extent. These contributions can be important, depending on meteorological situations, over a wide range of distances. Therefore, it seemed worthwhile to try to validate the model of the single elevated point source (steady state Gaussian plume).

II. Elevated Point Source Model Validation

After some discussions and looking into the availability of possible data sets, it turned out that the data most suitable for this purpose are those from TVA electric power generating plants and especially those from the Paradise Steam Plant. This is located on the west bank of the

Green River in Muhlenberg County, near the village of Paradise in Western Kentucky. The plant has three units, of which units 1 and 2 have a capacity of 704 MW and unit 3 of 1150 MW. The stack heights are 183m, 183m, and 244m, respectively.

A. The facts which make this data set suitable are as follows: Through 1971 the following data are available for this plant:

1. The daily SO_2 output data for each unit calculated from the daily coal consumption and a weekly average sulfur content of the coal. Since the coal used comes only from adjacent coal fields, the sulfur content is relatively constant.
2. The hourly total MW data for the sum of the three units.
3. Meteorological hourly data. These consist of wind speed and wind direction at two different heights (13.4 m and roughly 110m above the ground), vertical temperature differences between three different heights, surface temperature, surface pressure, amount of rainfall, total and solar radiation.
4. Hourly SO_2 concentration data for 6 stations continuously through 1971. These stations are located downwind of the prevailing wind direction and range in distance fram ca. 2 to 17 miles.
5. Empirical relationships for the dependence of stack gas exit velocity on MW load. The exit temperature of the gases does not vary significantly with load and was therefore assumed to be constant.

B. Furthermore, there seems to be no background concentration (SO_2 or other substances to which the conductivity method of concentration measurement may be sensitive) in the area and the surroundings of the site are relatively even compared with the effective height of the plume

The procedures of calculating the surface concentrations at a receptor point are the following:

1. Determine the output data
    a. The hourly SO_2 output by multiplying the daily SO_2 output of the respective unit with the ratio of total hourly MW load to the daily average total MW load. Result: Hourly SO_2 source strength in g sec^{-1}.
    b. The hourly exit velocity of each unit by multiplying the total hourly MW load with a regression factor (supplied by TWA) times the ratio of the daily unit source strength to the sum of the three unit source strengths. Result: Exit velocity in m sec^{-1}.
    c. Take the exit temperature of the unit (unit 1 and unit 2 413.2°K, unit 3 402.2°K). Result: Exit temperature in °K.
    d. Compute the effective source height by using Brigg's formulation (Atmos. Env. 6, 507-510 (Jul. 72)) for unstable-neutral and stable surroundings. The stability is determined from the measured temperature differences

between 1m and 110m above ground. The wind speed used is measured at 110m. Result: Effective source height in m.

2. Use the hourly Meteorological Data:

   a. If the wind direction averaged over one hour at 110m is outside a sector, which is given by the bearing from true North with respect to the source of the receptor station +180° ± 45°, then the concentration at this receptor point is assumed to be zero.

   b. If the wind direction is within this sector, the concentration is calculated by using the bivariate normal distribution for the concentration:

      (1) The wind direction at 110m and the bearing and distance of the receptor to calculate the x,y-coordinates of the receptor.

      (2) The temperature difference between 110m and 1.5m and the wind speed at 13m for determining the stability class by the following scheme:

U_{13m} m sec^{-1} \ $T_{1m-110m}$ °C	> 2.	1.9-1.3	1.2-.8	.7-.2	.1--.5	≤ 1.6
≤ 5	A	B	C	D	E	F
> 5	B	C	C	C	D	E

This scheme was set up intuitively by relating the C-class to adiabatic stratification and the extreme values of observed differences to classes A and F, respectively.

(3) The standard deviations in the vertical and horizontal direction σ_y and σ_z are used according to the above scheme and

(a) Pasquill's original σ-dependencies on distance and stability classes.

(b) Pasquill's new power law dependencies obtained from F. B. Smith's K-theory computations. The use of these unpublished values is gratefully acknowledged by the author.

(4) The wind speed at 110m

c. After the concentration for this measured wind direction is computed, the wind direction is arbitrarily changed to wind direction ±10°, ±20°, ±30° and the concentration is computed again. This is done in order to study the influence of changing wind direction with height.

d. The concentration which is closest to observed concentration is noted.

e. These 8 concentrations (7 computed ones, the best estimate of the 7 and one observed) are written on tape.

For all 8 data sets the frequency distributions are calculated and compared.

III. Results

The results, which have been obtained so far and which are not complete, are as follows:

A. Mean values: The ratio of observed to calculated mean values averaged over the year ranges for the six different stations from 0.55 to 1.94 for the original σ-values, from 0.44 to 1.31 for the more recent data set mentioned above. There is a systematic variation for this ratio: the mean values are calculated too high for small distances, and too low for large distances.

B. The standard error of estimate between observed and calculated concentrations is approximately 3 to 4 times the mean values; all values of this quantity are 10-20% smaller for the original σ-values than for the new ones.

C. The correlation coefficient between the logarithm of concentrations varies between 0.18 and 0.28. There is no systematic variation with distance. If the arbitrarily changed wind direction is considered and the concentration is picked in each case which is in relatively best agreement with the observed one, then the correlation coefficient between the logarithm of the concentrations increases considerably and ranges from 0.47 to 0.65.

D. If the cumulative frequency of the logarithm of concentrations is plotted on probability paper it is evident, that for short distances the calculated concentration frequency is too high for high concentrations and too low for low concentrations, whereas for the more distant stations the calculated cumulative frequencies are lower than the observed distribution.

E. When changing the wind direction arbitrarily and noting for which of the changed wind directions best agreement is obtained between observed and calculated concentrations, it was anticipated, that there would be a systematic, stability dependent deviation. This was found for a subset of observations for one week, when best agreement was obtained when the measured wind direction at 100m height was changed to wind direction +20° (to the right), indicating that the turning of the wind with height over the height of the plume was being felt by the surface concentration field. For the whole data set this could not be found, not even when the data were subdivided into daytime (10-16 hrs) and nighttime values (22-06 hrs).

The above findings have led to the conclusion that the scheme which relates vertical temperature differences to stability classes is not optimal. A new scheme is being devised and the calculations will be repeated. It is hoped that better agreement will be achieved.

Chapter 37

SOME VIEWS ON MODELING DISPERSION AND VERTICAL FLUX

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

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Some views on modelling dispersion and vertical flux

by F. Pasquill and F.B. Smith

In conventional dispersion modelling we are concerned with semi-empirical predictions of the vertical (σ_z) and lateral (σ_y) spread of a point source plume, and of the effective height of the source in the case of hot chimney effluent. The resultant errors in concentration which arise in practice from the combination of the separate errors in estimating these three parameters have been discussed previously (Pasquill 1973).

For surface releases and short range (ca 1 km) over uniform terrain experience suggests that each of the spreads might be estimated (semi-empirically) with a r.m.s error of 10-15% for individual occasions with sampling over some minutes at least. For elevated sources of given height the most important error is in estimating the distance (x_m) of maximum concentration, (implying an error in estimating σ_z), and may be ± 35% (r.m.s) in unstable conditions. This error largely determines the final error in the magnitude (C_m) of the ground-level maximum concentration. These r.m.s errors are increased still further when the effective height of the source has to be calculated semi-empirically and then are estimated to reach around 50% for the hourly average ground-level maximum concentration. An even more dramatic increase in error (to near 100%) appears when the interest is in the concentration at a fixed receptor within a multiplicity of sources, presumably a consequence mainly of the combination of all the foregoing errors with errors in the assumed wind direction.

In considering these errors it is worth remembering that the conventional approach, with plume geometry specified in terms of σ_y and σ_z, implicitly contains the basic physical principle represented in the conservation expression, e.g. for the two-dimensional (line source) case

$$\bar{u}\frac{\partial C}{\partial x} = \frac{\partial F}{\partial z}$$

where F is the vertical turbulent flux. $C(x,0)$ therefore has to be evaluated through $\partial F/\partial z$ at $z = 0$. In certain simple situations when it is valid to assume that u is constant with height and that vertical profiles are similar irrespective of distance (i.e. a universal function of z/σ_z) it follows that $C(x,0) \propto (\bar{u}\,\sigma_z)^{-1}$.

The value of σ_z may be obtained by any one of several methods, one of which may in fact be solving directly a simplified integrated form of the conservation equation itself. The alternative methods also imply, albeit implicitly, a conservation of material C and it is worth re-emphasising that essentially the so-called plume-model approach simply represents a convenient simplification of the problem of finding a general solution which, although it may introduce an error (which is often only marginal), is fundamentally equivalent to solving the full basic diffusion (i.e. conservation) equation.

However in a more complex situation such as over a heterogeneous city-complex this simple approach may be acceptable no longer and we are forced back to a direct solution of the fundamental equation :

$$u\,\frac{\partial C(x,0)}{\partial x} = \left(\frac{\partial F}{\partial z}\right)_{z=0}$$

Much interest is now being developed in modelling of the flow field itself, and in the avoidance of the suspect gradient-transfer theory, the implication being that it should be possible thereby to reduce the errors in conventional dispersion modelling. But even for a prime flow property such as wind direction it has not yet been established how far flow-modelling may be expected to succeed in important practical circumstances, such as those mentioned above of a large urban-industrial area with variations in topography, aerodynamic roughness and buoyancy effects. For the more complex effects which determine the dispersion of injected material it seems even more a matter of wishful thinking.

The formulation of higher-order equations for turbulent transport in the hope of avoiding the gradient transfer approach is no doubt an important step, but closure approximations and assumptions are still required. We consider it important to keep these in mind stage by stage, and to design observational tests of the most searching nature, rather than to construct a whole closed hierarchy of equations and test the net effect against a whole practical survey in a multi-source situation.

As an example of what we have in mind we offer the following preliminary considerations of the vertical flux in the one-dimensional time-dependent case. Physically, for example, this corresponds to the non-steady evaporation from a uniform effectively infinite area of evaporating surface, and is also the time-analogue of the advective build-up of pollutant concentration over an area source with non-uniform emission.

As we have noted, the interest is especially in $\left(\frac{dF}{dz}\right)_{z=0}$. Consider this quantity F ($= \overline{w'C'}$) for passive material (concentration $C = \overline{C}+C'$) in terms of the 2nd order equation (e.g. see Donaldson 1973). The full equation in the one-dimensional context is

$$\overline{w}\,\frac{\partial\overline{w'C'}}{\partial z}^{(1)} + \frac{\partial\overline{w'C'}}{\partial t}^{(2)}$$

$$= -\overline{w'^2}\,\frac{\partial\overline{C}}{\partial z}^{(3)} - \overline{w'C'}\,\frac{\partial\overline{w}}{\partial z}^{(4)} - \frac{\partial}{\partial z}\overline{w'^2C'}^{(5)}$$

$$-\frac{1}{\rho}\,\frac{\partial(\overline{p'C'})}{\partial z}^{(6)} + \overline{\frac{p'}{\rho_0}\,\frac{\partial C'}{\partial z}}^{(7)}$$

$$+\, g\,\frac{\overline{C'T'}}{T_0}^{(8)} + \nu\,\frac{\partial^2\overline{w'C'}}{\partial z^2}^{(9)} - 2\nu\,\overline{\frac{\partial w'\,\partial C'}{\partial x_i\,\partial x_i}}^{(10)}$$

Simplifying to zero-divergence of the flow terms (1) and (4) are eliminated. The pressure fluctuation terms (6) and (7) are of unknown magnitude but for a passive property it is difficult to see any reason for important magnitudes. The 'molecular' terms (9) and (10) are also of unknown significance - presumably (10) is a 'decorrelation' term analogous to the dissipation of turbulent fluctuations of velocity, but estimation thereof is at present problematical.

We see therefore that even with a simplified situation the position as regards solving the equation for $\overline{w'c'}\,(z)$ as a function of time is not straightforward and the best we can now do, hopefully, is to consider the equation as essentially reduced to

$$\underset{(2)}{\frac{\partial \overline{w'c'}}{\partial t}} = \underset{(3)}{-\,\overline{w'^2}\frac{\partial \bar{c}}{\partial z}} \underset{(5)}{-\,\frac{\partial \overline{w'^2c'}}{\partial z}} \underset{(8)}{-\,\frac{g\,\overline{c'T'}}{T}} \underset{(10)}{+\ \text{'decorrelation'}}$$

A useful next step would be to examine the magnitudes of the terms (2), (3), (5), and (8) observationally, and to consider further and theoretically term (10). For the observational study we could use humidity mean profile and humidity/vertical component fluctuations at two or more low heights above a near-ideal large area of grassland, in the morning regime of build-up of evaporation.

Some estimates may be made without further ado for the terms (2) and (3), for despite the suspicions about the gradient-transfer approach we know that realistic estimates of $\overline{w'c'}$ are thereby provided for water vapour at low heights and we can also make quite good estimates of $\overline{w'^2}$ at low height, e.g. from a specification of z_0 and u_*. Following this line in terms of humidity profile data and evaporation estimates published by one of us (Pasquill 1949) we find that typically in the forenoon rise of rate of evaporation term (3) is 10^4 times term (2) at a height of roughly 0.5 metres.

It is of course evident from the typical diurnal trend in evaporation that shortly after noon the rate of evaporation is a maximum, while $\frac{\partial \bar{c}}{\partial z}$ is large, and it is then obvious that term (2) is a negligible term in the balance. However, what was not immediately obvious is the typically low relative order of this term in the important morning phase of the diurnal cycle.

In our present context this has an immediately disconcerting implication if we are set on the course of estimating $F(z,t)$ without using the gradient-transfer assumption in a 1st-order closure. From the results above it would appear that assumptions made about the component terms in the 2nd-order equation (e.g. the 3rd-moment term at (5)) must be correct to the order of 0.01 per cent !! We do not have immediately any numerical data for the analogous case of $\frac{dF}{dx}$ over a large area source with source strength q building-up to a maximum at some position. However, at first sight there seems no reason to expect radically different relative magnitudes of the terms which determine $\frac{dF}{dx}$.

To summarise, the purpose of our discussion is to bring out three main points :

1. Conventional dispersion modelling has fairly clearly defined limitations and inaccuracies.
2. In its most practical form (plume modelling) the basic 1st-order conservation equation is fully implied.
3. Use of 2nd-order conservation equations, to circumvent the objections to closure at the 1st-order, may require closure assumptions which would have to be valid to an accuracy which we cannot visualise ever being attained.

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Chapter 38

FURTHER COMPARISON OF URBAN AIR POLLUTION MODELS

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Roskilde, Denmark
4-6, June, 1974

Comparisons of the ATDL simple urban diffusion model with the outputs of other models and with urban pollution data, described in a previous report to this group (Gifford, 1973), have continued. Some recent results will be summarized briefly below. The derivation of our model was given in some detail in the reference.

The comparisons reported previously consisted of pairs of correlations of the output of the simple model and other models with data. Many urban pollution models have been applied to Los Angeles County pollution data because the available data from several limited observational periods there are quite complete. A problem with model-data comparisons of this type is that it isn't clear exactly in what sense the correlation coefficients involving a number of models can legitimately be compared with one another. In particular space correlations for different arrays of sampling locations are strongly influenced by the particular sampling pattern involved. Thus it is desirable, in order to compare many models on a common basis, to work as much as possible from the same data base.

Problems of this kind have influenced a study by Nappo (1974) in which a number of urban models, applied to the same Los Angeles air pollution problem, are being compared. Figures 1 and 2 display some preliminary results from this study. The pollutant is in each case carbon monoxide. In addition to the ATDL simple model and various other published modeling results, persistence has also been included. In Figure 1, for each model, the plotted point indicates two correlations: 1) the correlation of the predicted with the observed time pattern of CO concentration, for data that have been averaged over all the eight CO sampling stations in Los Angeles County; and 2) the correlation of the predicted with the observed space pattern of CO concentration, for data that have been averaged over the (12 hour) time period at each station. The basic concentration, source strength, and wind data are those previously presented and discussed by Hanna (1973a).

In Figure 2 another statistic based on the same data and space and time averaging is presented for each model. This is the standard deviation of the ratio of the predicted to the observed concentration values at each station for each hour.

In my previous report to you (Gifford, 1973) I presented a series of correlations which indicated a generally favorable level of performance of our simple model, compared to various other, more complex models. Correlations of either space or time concentration patterns for the simple model were generally as high as or a bit higher than those for the complex models. For the particular Los Angeles CO-pollution data set, however, Figures 1 and 2 seem to show a more complicated picture. The simple model (ATDL-1) provides, in Figure 1, a resonably high correlation, $\overline{R(t)}^{s}$, of the space-averaged time-concentration patern, as high as most of the other models. The corresponding space-correlation, $\overline{R(s)}^t$, of the time-averaged values is however rather low in this case, both in absolute value and relative to that of other models. Of course these models in almost all cases represent years of development and adjustment involving the same data. In no case (except for the predictions of the simple ATDL model and of persistence) could these results be accepted as defining the final model performance level without verification on independent data. But it seems unlikely that future, independent testing would modify radically the pattern of results in Figure 1.

The situation displayed in Figure 2 is of even more concern. It appears that the detailed, hour-by-hour predictions of the simple model for each station exhibit considerably more variability than do all other models, including persistence. Mr. Nappo has proposed what is probably the correct interpretation. Examination of the data (see Hanna,1973) show that the excessive variability and "over-prediction" exhibited by the simple model almost always occurred when the observed wind speeds were low. This happened mainly at locations (Burbank, West L. A., Reseda) that the surface wind field analysis (see Roth, 1971) indicated to be near areas of horizontal convergence which, of course, the simple model does not consider.

The remedy is a simple one. If the wind speeds for each hour are first averaged over all stations prior to forming the time-pattern statistics, and for each station are first averaged over all the hours prior to forming the space-pattern statistics, the points labeled ATDL-2 on Figures 1 and 2 are obtained by application of the simple model. This modification results in a much more satisfactory performance level and is in fact a more reasonable interpretation of the transport wind speed, u, that is the required input to our model.

In discussion during the previous meeting of this group, Dr. Olsson suggested that the performance of a simple model such as ours, applied to a short-period pollution forecast, could be improved by including a correction to account for the diurnal march of stability. This is accomplished in our model simply by modifying the stability-dependent parameter c. To check on this suggestion, the time-concentration pattern of the previous version of our model (ATDL-2) was arbitrarily modified. (The space-pattern statistics are of course not affected). The modification consisted in (arbitrarily) reducing the value of c by 50% between 0800 hrs. and 1200 hrs. and then increasing it slightly after 1300 hrs. The results appear in Figures 1 and 2 as the points labeled ATDL-3. These are seen to provide a considerable improvement over the previous space-averaged time-pattern statistics, just as Dr.Olsson supposed would be the case.

Of course it would be desirable, in the first place, to introduce the diurnal stability influence on c on some basis related to the observed micrometeorological fields and to its definition, for which see Gifford (1973). Then too, of course, this and the previous modification should be verified on independent data (as should, also, the developmental results of all the other urban models). Nevertheless it is interesting that such simple, reasonable adjustments of the ATDL model result in sizeable improvements in data correlation. As to the future, we plan to continue model-data comparisons in an attempt to define an optimum regional-scale transport and diffusion model which we need for many applications. At the same time we are continuing development of the chemical-reaction model described by(Hanna, 1973b).

Acknowledgement

This research was performed under an agreement between the Atomic Energy Commission and the National Oceanic and Atmospheric Administration.

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Figures:

Figure 1. Correlations, for the indicated models, of observed vs. predicted concentrations for Los Angeles carbon monoxide air pollution data; $\overline{R(t)}^s$ refers to time-pattern correlations of space-averaged data; $\overline{R(s)}^t$ refers to space-pattern correlations of time-averaged data.

Figure 2. Standard deviations, for the indicated models, of the ratio of predicted to observed carbon monoxide concentrations at Los Angeles air pollution monitors; $\overline{\sigma(t)}^s$ refers to space-averaged data and $\overline{\sigma(s)}^t$ refers to time-averaged data.

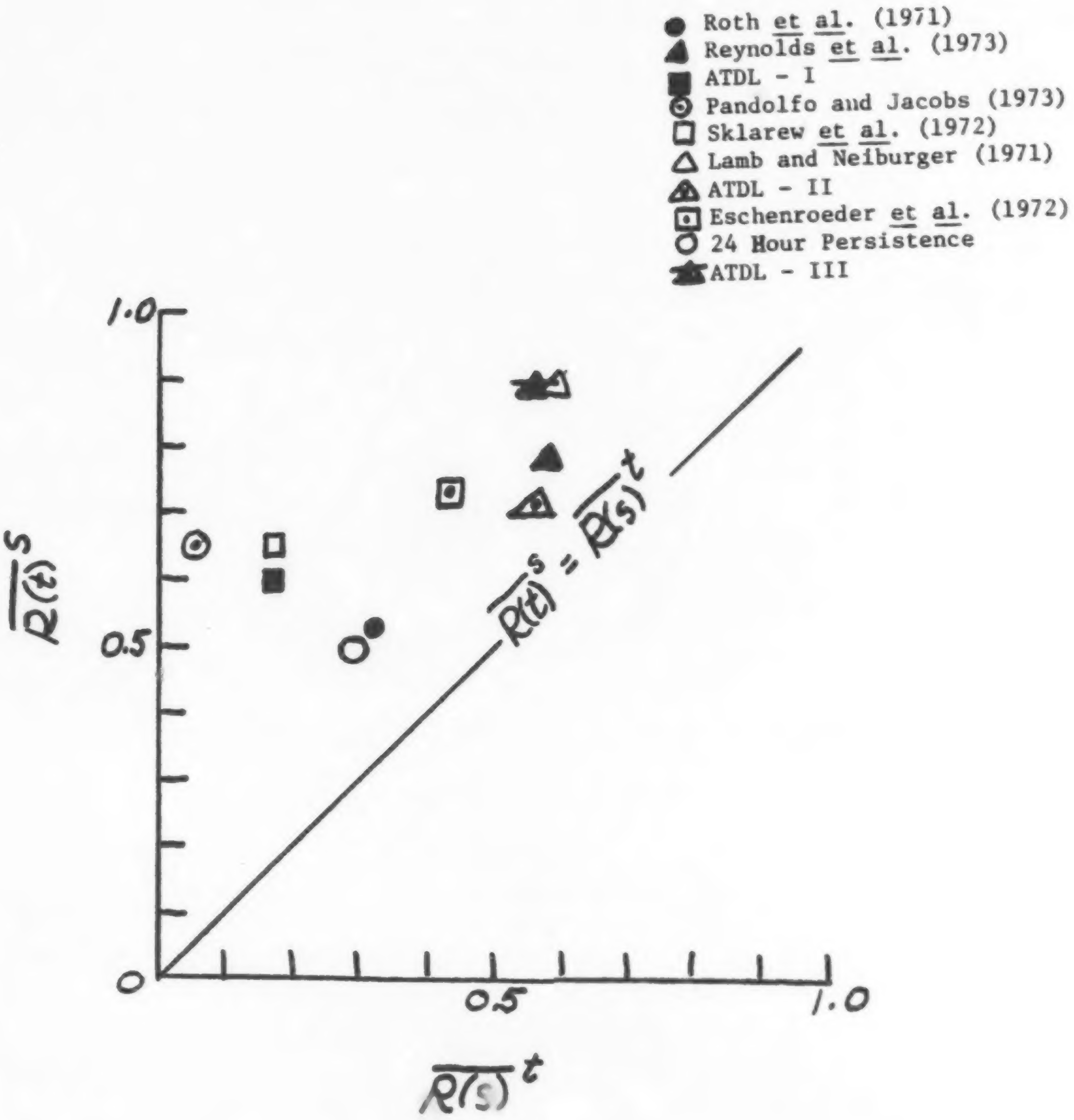
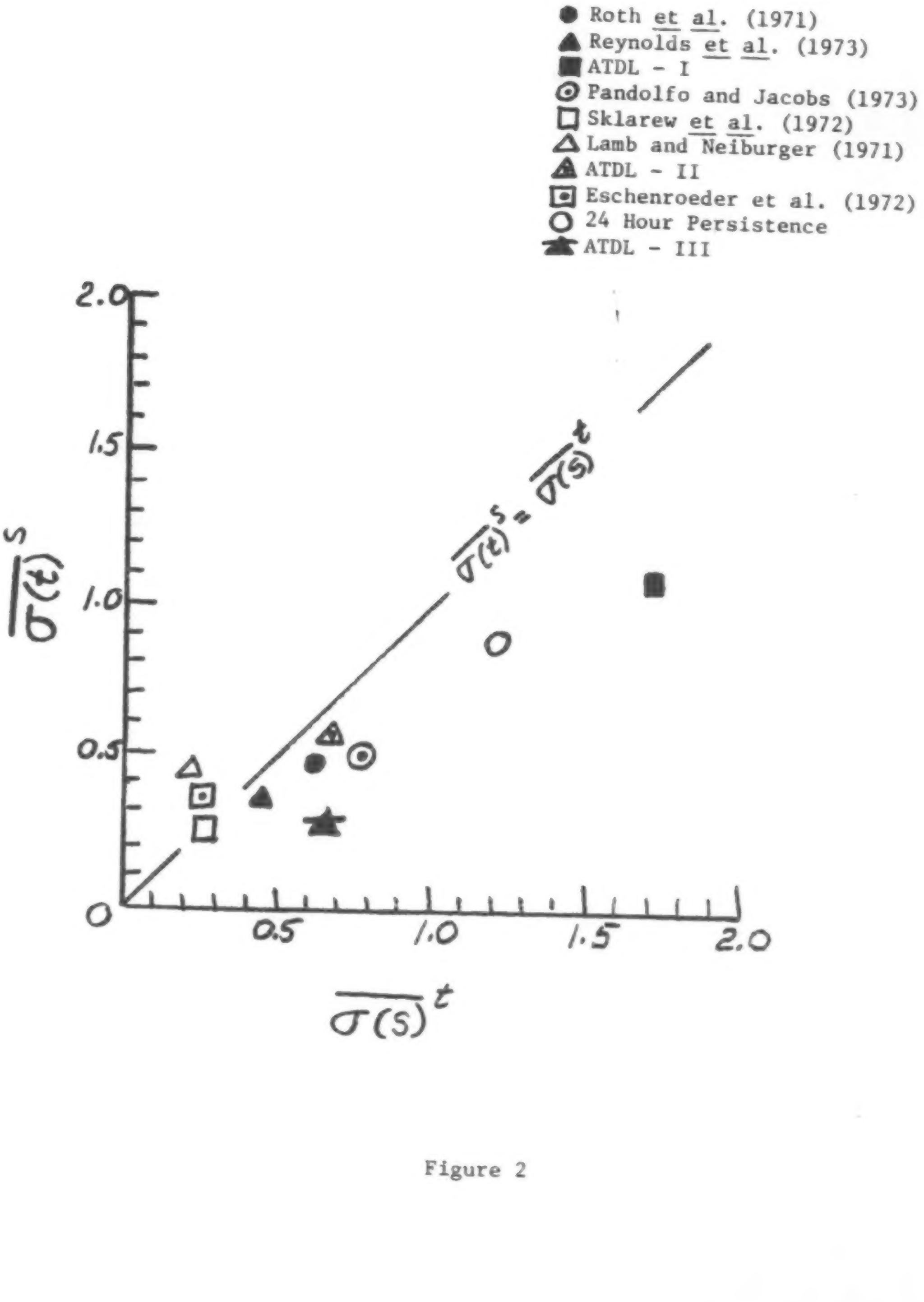

● Roth et al. (1971)
▲ Reynolds et al. (1973)
■ ATDL - I
⊙ Pandolfo and Jacobs (1973)
☐ Sklarew et al. (1972)
△ Lamb and Neiburger (1971)
△ ATDL - II
▣ Eschenroeder et al. (1972)
○ 24 Hour Persistence
★ ATDL - III
1.0
0.5
0
0.5
1.0
$\overline{R(t)}^s$
$\overline{R(s)}^t$
$\overline{R(t)}^s = \overline{R(s)}^t$

Figure 1


● Roth et al. (1971)
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⊙ Pandolfo and Jacobs (1973)
☐ Sklarew et al. (1972)
△ Lamb and Neiburger (1971)
ATDL - II
Eschenroeder et al. (1972)
○ 24 Hour Persistence
★ ATDL - III
$\overline{\sigma(t)}^s = \overline{\sigma(s)}^t$
$\overline{\sigma(t)}^s$
$\overline{\sigma(s)}^t$
0
0.5
1.0
1.5
2.0
0.5
1.0
1.5
2.0

Figure 2

Chapter 39

RÉSUMÉ OF ACTIVITIES OF THE NATO/CCMS EXPERT PANEL ON AIR POLLUTION MODELING, 1970-74

by

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5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

INTRODUCTION AND OBJECTIVES

The activities of the NATO/CCMS Expert Panel on Air Pollution Modeling date back to 1970, during the first year of the Pilot Study on Air Pollution. An ad hoc Panel was then established, under the chairmanship of Mr. R. A. McCormick (U.S.A.), and with representation from the pilot and co-pilot countries (U.S.A., Turkey, F.R.G.) and observers from France, The Netherlands, and Italy.

During Phase I of the Pilot Study which was primarily concerned with sulfur oxides and particulate pollutants, the primary function of this Panel was to examine and propose appropriate air quality simulation models for application to the ongoing air pollution studies in Ankara (Turkey), Frankfurt (F.R.G.), and St. Louis (U.S.A.). The model applications were to include not only comparisons with observational data on air quality but also, for urban planning purposes, the prediction of the future air quality for 1990, based on projections of emissions and demographic changes. In addition, the Panel was to address itself to a review of progress on the mathematical modeling of air quality and the data requirements for optimum model development and application.

Air quality simulation modeling has attracted widespread attention in recent years and has been in an exceptionally rapid state of development. Because of the rapid advances in techniques and the diversity of the applications of modeling it was soon apparent that there might be great merit in extending the participation at the Panel meetings, by calling together the most active practioners of the modeling art. This would provide an opportunity for informal give-and-take of the latest information on modeling and closely related topics. It was also considered to meet an obligation to keep users of our products informed as to their current nature and quality. Furthermore, it was consistent with a stated CCMS policy that information developed would be unclassified and generally available to other countries and organizations, both within and outside NATO. Participation at the later meetings of the Panel was therefore purposely enlarged to include representation well beyond the initial regular membership countries.

The first meeting* of the Panel was held on 9 October 1970 in Frankfurt, and was attended by fourteen participants representing the F.R.G., U.S.A., Turkey, The Netherlands, France, and Italy.

The second meeting was held 26-28 July 1971 in Paris, and was attended by seventeen participants representing the same countries.

The third meeting was held 2-3 October 1972 in Paris, and was attended by twenty-eight participants. It now included additional representation from Denmark, Sweden, Norway, United Kingdom, and Canada.

The fourth meeting was held on 28-30 May 1973 at Oberursel (F.R.G.) and was attended by forty-four participants representing a total of fifteen countries, namely, the F.R.G., U.S.A., The Netherlands, France, Italy, Denmark, Sweden, Norway, United Kingdom, Canada, Belgium, Australia, Israel, Greece, and Czechoslavakia.

A fifth meeting is planned for 4-6 June 1974, to be held at the Danish Atomic Energy Commission Research Establishment Risø, Roskilde,

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* This was proceded by an organizational meeting held in Paris on 29 May 1970 and attended by Messrs. R. A. McCormick (Chairman, U.S.A.), K. L. Calder (U.S.A.), E. Weber (F.R.G.), and H. Fortak (F.R.G.).

Denmark. It is hoped that this will include additional representation from Japan, Switzerland, Hungary, Spain, and the U.S.S.R. The fifth meeting will emphasize a new direction for future activities of the Panel and one that was first highlighted at the fourth meeting. This is concerned with improving the communications between the modeling scientist and the policy making user. The meeting will set the precedent for interfacing users and modelers.

A comprehensive list of the participants at the first four meetings, together with their affiliations, is provided in Appendix I to this paper.

Proceedings of the Panel meetings have been published under the auspices of the NATO Committee on the Challenges of Modern Society, 1110 Bruxelles, Brussels, Belgium, as follows:

2nd Meeting - NATO/CCMS Publication No. 5
3rd Meeting - NATO/CCMS Publication No. 14
4th Meeting - NATO/CCMS Publication No. 30

DISCUSSION TOPICS

A substantial number of technical papers relating to various aspects of air quality simulation modeling and related topics have been published in the Proceedings of the 2nd, 3rd, and 4th Meetings. Some indication of the variety of these topics may be seen from Appendix II of this paper, which contains the tables of contents for these three volumes. In the following we attempt to give only a brief indication of the main thrust of each meeting, and reference should be made to the Proceedings for further details.

1st MEETING, 9 OCTOBER 1970: FRANKFURT

The meeting reviewed a detailed U.S. technical report entitled "A Climatological Model for Multiple Source Urban Air Pollution" (see Proceedings of 2nd Meeting) that had been distributed in advance of the meeting. The model was proposed for application to the Ankara air pollution problem and offered the possibility of predicting the changes of air quality to be expected when the pattern of emissions was hypothetically and arbitrarily changed in anticipation of urban growth and development. The simple structure of the model permitted application in a wide variety of situations for which the more detailed input information required by sophisticated models would be unavailable. The Panel endorsed the application of this model for the Ankara problem and the same model would be used in the St. Louis study. There was also some discussion of the modeling techniques that were candidates for application to Frankfurt. These were adaptations of the Bremen model as earlier developed by Professor Fortak (F.R.G.). The question of compatibility of computer programs was also briefly discussed. Computer programs for various urban diffusion models that might be considered by the Panel would all be written in FORTRAN IV. This could, therefore, be readily applied by any of the participating countries without the need for major computer-program translation effort.

The Chairman indicated that the physical modeling (i.e. hydraulic and/or aerodynamic) of some aspects of urban air pollution might provide an alternative to mathematical modeling. In response Dr. Jacquet (France) said that the two approaches were really complimentary and that in France, construction of a large-scale wind tunnel had been proposed for this purpose. He would submit a detailed technical paper on this subject at the next meeting.

The Chairman raised the question of the influence of atmospheric physical and chemical transformations on urban pollution modeling and suggested it as a topic for discussion at the next meeting.

2nd MEETING, 26-28 JULY 1971: PARIS

This meeting included the presentation of papers and discussions (see Appendix B and Proceedings of 2nd Meeting) relating to the three primary topics: (a) the current status of the Ankara and Frankfurt air pollution modeling studies; (b) the possible applications of physical modeling using hydraulic and aerodynamic techniques in air pollution studies; and (c) the problems of physical and chemical transformations in air pollution modeling.

By special invitation to the meeting Mr. John A. Haines, of the Organization for Economic Cooperation and Development, briefly described the recent OECD cooperative plans for a comprehensive air pollution measurement survey to study long range transport of air pollution in Western Europe. This was primarily related to sulfur compounds in the lower atmosphere, but eventually would include measurements of acidity in precipitation.

The meeting concluded with a visit to the laboratories of the French National Meteorological Office at Magny Les Hameaux, and a conducted tour of the laboratories and discussion of water channel modeling experiments by Dr. L. Facy.

3rd MEETING, 2-3 OCTOBER 1972: PARIS

This meeting was intentionally enlarged beyond the regular Panel membership so as to accommodate a broader objective and to encourage a maximum exchange of ideas on a wide front between many of the most active contributors in the field of air quality simulation modeling. All the participants had been invited to submit, in advance, extended abstracts in English of the material that they would present. These were distributed prior to the meeting to provide a better basis for discussion (see Appendix B and Proceedings of the 3rd Meeting).

The agenda included specific items for the discussion on the status of ongoing modeling efforts for Cologne, Ankara, St. Louis, Frankfurt, Dusseldorf, and Milan, and an item on the criteria for the validation of air pollution prediction models. However, a major portion of the meeting was devoted to discussion of a miscellany of topics (see Appendix B) and presentation of papers by the various participating countries (U.S.A., F.R.G., Turkey, France, Italy, The Netherlands, Canada, United Kingdom, Denmark, Norway, and Sweden).

4th MEETING, 28-30 MAY 1973: OBERURSEL, W. GERMANY

Encouraged by the apparent success of the 3rd Meeting, the 4th was also one of wide participation. However, in contrast to the 3rd, for which participants were invited to submit prepared papers, the 4th comprised a series of five workshop sessions and extended over the entire three-day period. These workshops were on the following topics:

(a) Applications of modeling and users' needs.

(b) Validation of air quality simulation models.

(c) The role of regional air pollution studies in model development.

(d) The role of empirical-statistical modeling of air quality.

(e) Simplicity versus sophistication in air quality modeling.

A brief summary of the several workshop discussions and the introductory remarks of the chairmen of the sessions, together with some papers that were variously prepared as back-up information for the workshops, are given in the Proceedings of the 4th Meeting (see also Appendix B of this paper).

The workshop on applications and users' needs, that occupied the whole of the first day, very strongly emphasized the need for improving communications between the modeling scientist and the policy-making user, and pointed to the need for a joint user-modeler exchange such as is now being planned for the 5th Meeting.

FORTHCOMING 5th MEETING, 4-6 JUNE 1974: ROSKILDE, DENMARK

The first 1 1/2 days of the meeting will be devoted to a modeler-user workshop aimed at improving the communications between the modeling scientist and the user of air quality simulation models. For this purpose a number of users and decision makers are being especially invited to attend this meeting. The remaining 1 1/2 days will be devoted to a discussion of the following five topics:

(a) Development of a common data base for air quality modeling.

(b) Validation of air quality simulation models.

(c) Short-term and real-time modeling.

(d) Modeling of complex topographic effects.

(e) Recent developments in air quality modeling.

APPENDIX I

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APPENDIX II

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PROCEEDINGS OF THE FOURTH MEETING OF THE EXPERT PANEL ON AIR POLLUTION MODELING

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Chapter 40

COMMENTS ON MODELER-USER CONFERENCE

by

W. Simmons
California Air Resources Board

5th Meeting NATO/CCMS Expert Panel
on Air Pollution Modeling

Danish Atomic Energy Commission Research Establishment Risø
Roskilde, Denmark
4-6, June, 1974

STATE OF CALIFORNIA—RESOURCES AGENCY RONALD REAGAN, Governor

AIR RESOURCES BOARD
1709 – 11th STREET
SACRAMENTO 95814

July 1, 1974

Mr. Ken Calder
Environmental Protection Agency
Meteorology Laboratory
Research Triangle Park, N.C. 27711

Dear Mr. Calder:

Subject: Fifth Meeting of NATO/CCMS Expert Panel on Air Pollution Modeling

You have asked me to submit to you my comments on the Modeler/User Conference so that they might be considered for inclusion in the written proceedings of the meeting. I offer the following rather unrelated observations:

1. "Users" (policy makers) should have at least the following basic understanding of models:

    a) What the basic models are;

    b) The many ways they can be used; and

    c) The limitations of models, particularly their reliability, or more precisely the extent to which each has been validated.

2. The reliability needed depends upon its use. Thus, a monitoring network can be established from a model which is not highly reliable. This is true for two reasons; the placement of monitoring stations can be checked out empirically and, more importantly, an error is not costly. As the use becomes more critical, error becomes more costly, and so reliability must be higher. If a control strategy for a particular pollutant is based on a model and the model is in error, the pollutant may be over controlled leading to unnecessary expense or under controlled leading to possible health hazards. The most critical use of a model is for abatement of episodes, viz., basing emergency action on a model's prediction. Shutting down industry and/or restricting movement of people has a

very high economic and social impact. It also has a very high political impact if the alert was called either too early or too late, or not at all. Erroneously calling an alert might well be finis for the model and the user. Users must understand this interrelationship.

3. Models need to be validated in a manner which is consistent with their probable use. Usually control strategies, and certainly emergency abatement actions, are based on worst-case situations, and the models need to be validated that way. For example, I have seen validation runs of oxidant models which began at 6 a.m. and ended at 3 p.m. High oxidant readings occur between 3 p.m. and 6 p.m. Thus, to me as user, I would be reluctant to use, for the two situations given, a model which has been validated up to 3 p.m., but no later.

4. At the meeting several people stated that the modeler needs to be involved in the decision-making process. I would agree with this statement generally, but with the following understanding. The involvement needs to occur first with the modeler informing the user of the various uses and the limitations of the models (point 1, above). Second, the modeler's input in the decision-making process need not be any greater than any other expert's input into a decision-making process where the process involves the use of technical information. In other words, I do not believe that modelers need be involved in decision-making any more so than other experts are needed in a particular situation.

5. It is evident that the Gaussian model is sufficiently developed and validated for wide use. However, other models, particularly those designed for oxidant, have a long way to go. Fortunately, progress appears to be rapid.

6. The modeling conference was useful to me mainly because it forced me to learn an area of pollution control with which I was relatively unfamiliar prior to my invitation to the meeting. In other words, to me the conference was useful because it forced me to learn about modeling before, during and after the meeting.

   However, I doubt if I was useful to the conference. I think this was true for several reasons:

   a) There were few users present and they were not identified early.

   b) Often the users were not specifically addressed.

   c) The format prevented, mainly through time limitations, the useful discussion which I think could have developed and which I had expected. What discussion did develop tended to be between modeler and modeler, not modeler and user.

d) This type of conference, or at least the scale of attendance at this type of conference, perhaps is the wrong way to bring the modeler and user together. This should probably occur at the local level so that the user may concentrate on his own problems. It is up to the modeler to bring to the user a broad background and current information on all the models and their use; then the modeler can furnish information as needed.

7. My only serious personal regret about the meeting is that more time was not spent on oxidant modeling; or rather I was sorry that I had not made personal arrangements to stay through the balance of the meeting, which dealt with oxidant to a greater extent.

I wish to thank EPA for making my participation possible.

Sincerely,

William Simmons
Executive Officer

cc: Dr. K. Jones, EPA, Washington, D.C.